VisTrails: A Python-based Scientific Workflow and Provenance System

David Koop

University of Utah and VisTrails, Inc.

VisTrails - Visual Workflow Programming

```
import vtk

data = vtk.vtkStructuredPointsReader()
data.SetFileName("../examples/data/head.120.vtk")

contour = vtk.vtkContourFilter()
contour.SetInput(data.GetOutput())
contour.SetValue(0, 67)

mapper = vtk.vtkPolyDataMapper()
mapper.SetInput(contour.GetOutput())
mapper.ScalarVisibilityOff()

actor = vtk.vtkActor()
actor.SetMapper(mapper)

cam = vtk.vtkCamera()
cam.SetViewUp(0,0,-1)
cam.SetPosition(745,-453,369)
cam.SetFocalPoint(135,135,150)
cam.ComputeViewPlaneNormal()

ren = vtk.vtkRenderer()
ren.AddActor(actor)
ren.SetActiveCamera(cam)
ren.ResetCamera()
renwin = vtk.vtkRenderWindow()
renwin.AddRenderer(ren)

style = vtk.vtkInteractorStyleTrackballCamera()
iren = vtk.vtkRenderWindowInteractor()
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iren.Initialize()
iren.Start()
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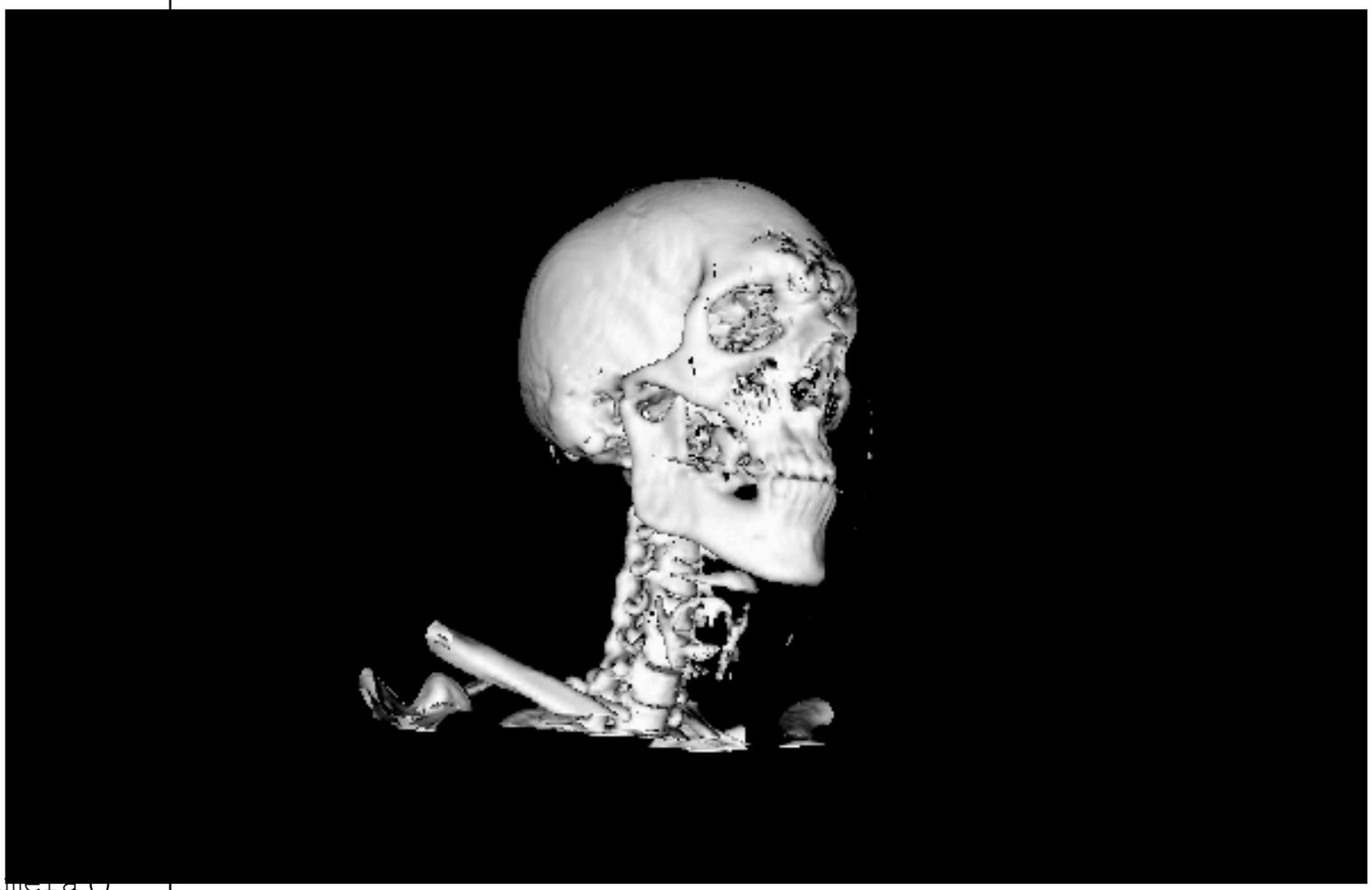
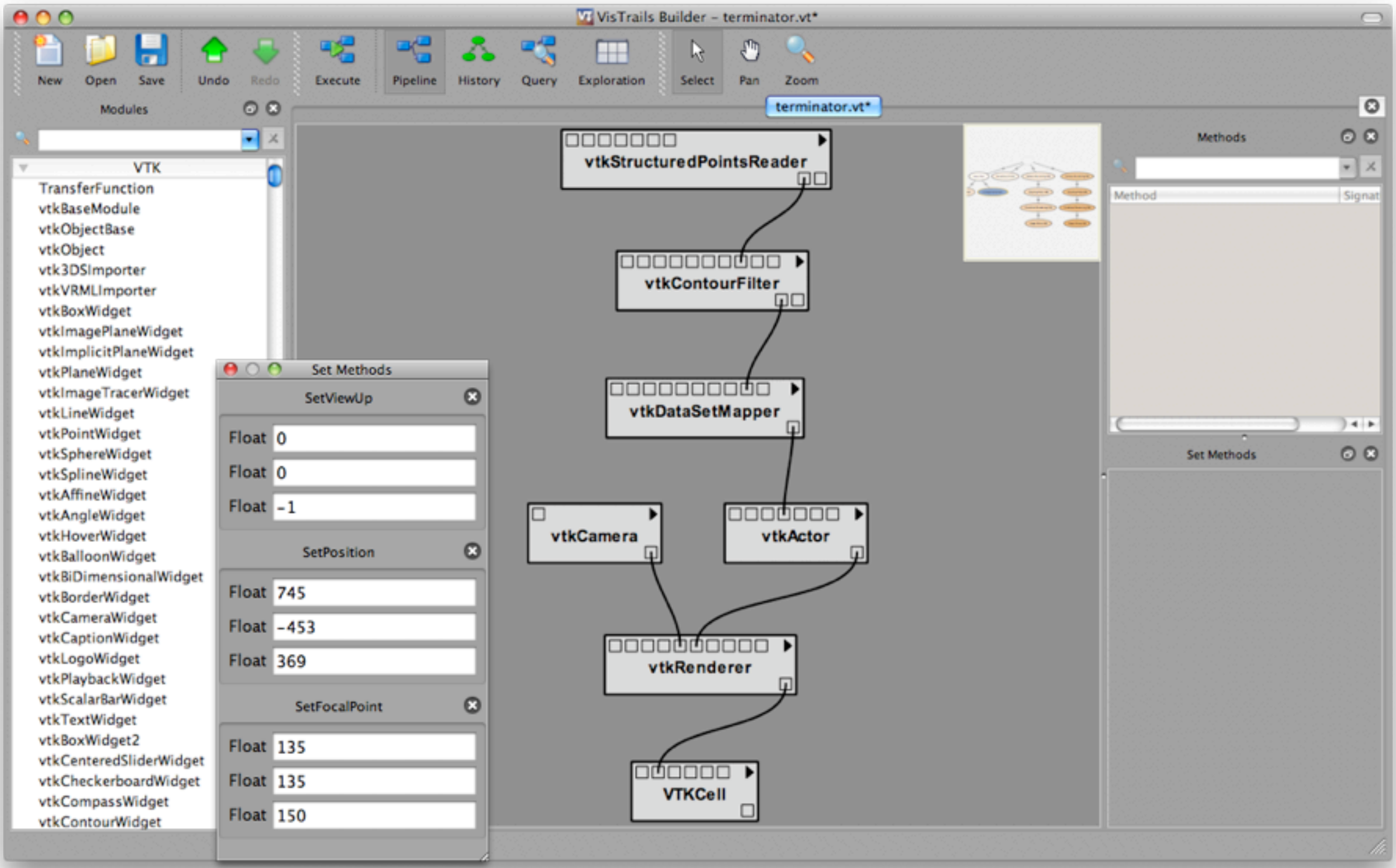
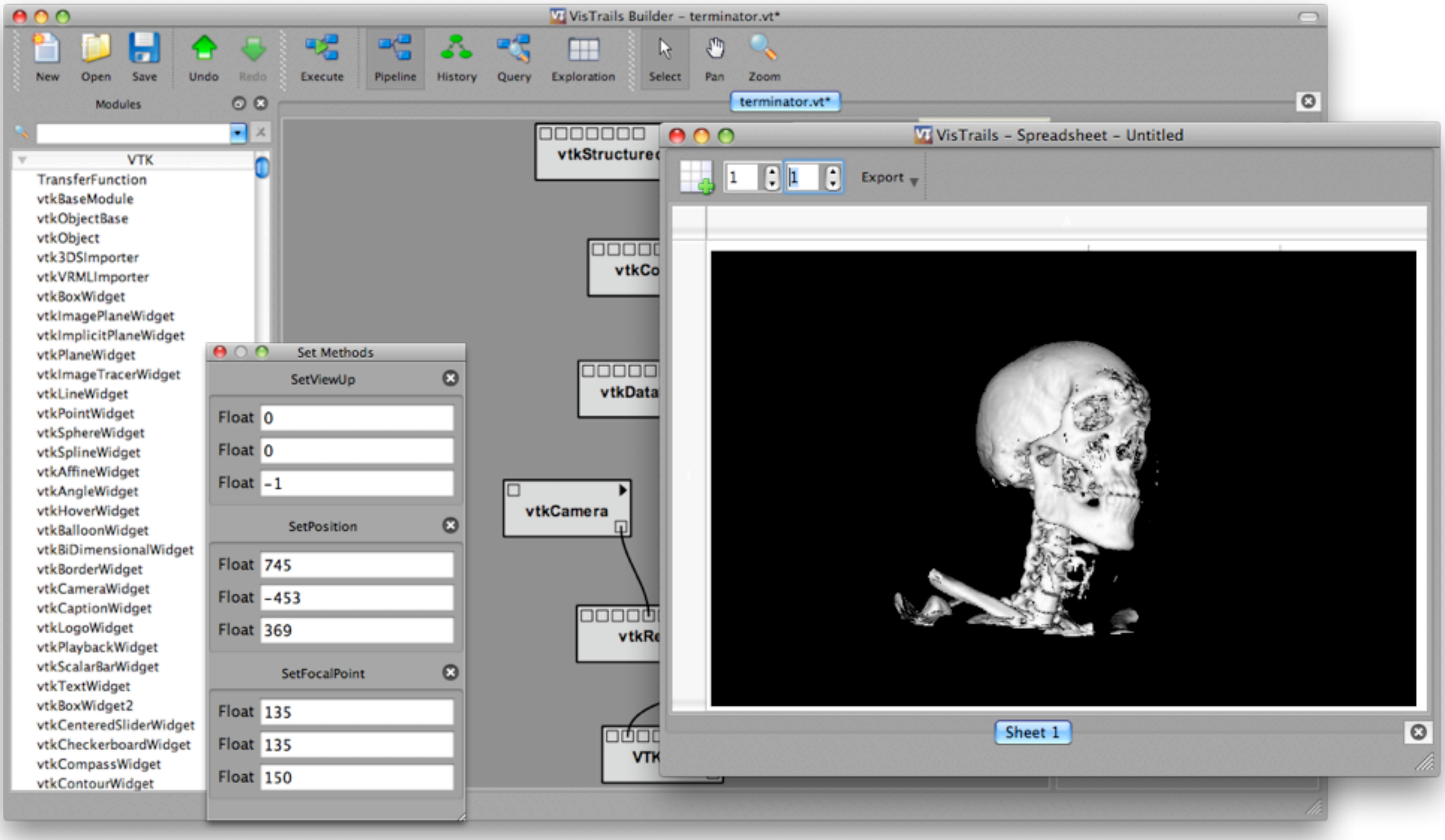


VisTrails - Visual Workflow Programming



VisTrails - Visual Workflow Programming



Friday, February 19, 2010

Structure Adds Value

1. 

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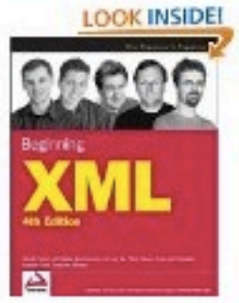
2. 

Beginning XML, 4th Edition (Programmer to Programmer) by David Hunter, Jeff Rafter, Joe Fawcett, and Eric van der Vlist (**Paperback** - May 21, 2007)

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Excerpt - Front Matter: "... Beginning **XML** 4th Edition ..."
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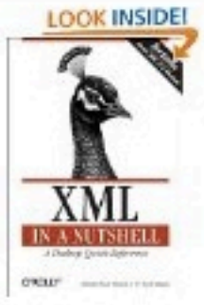
3. 

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Structure Adds Value


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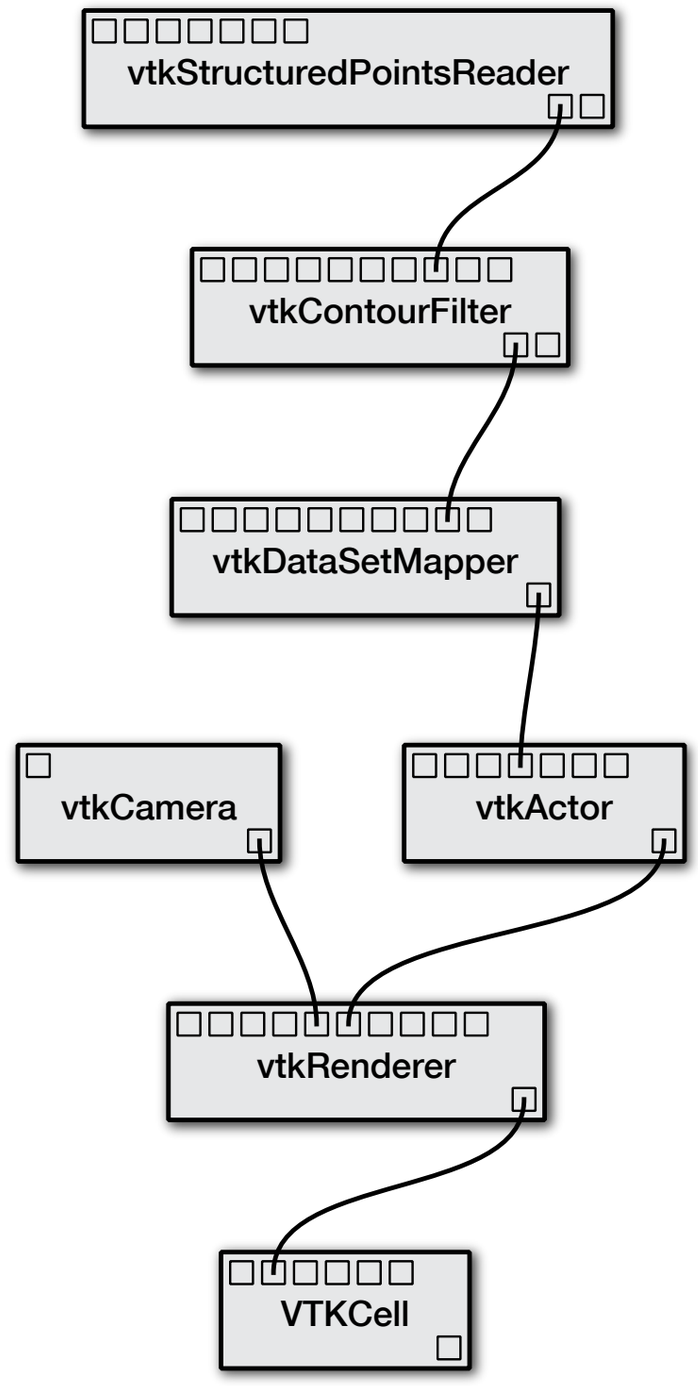
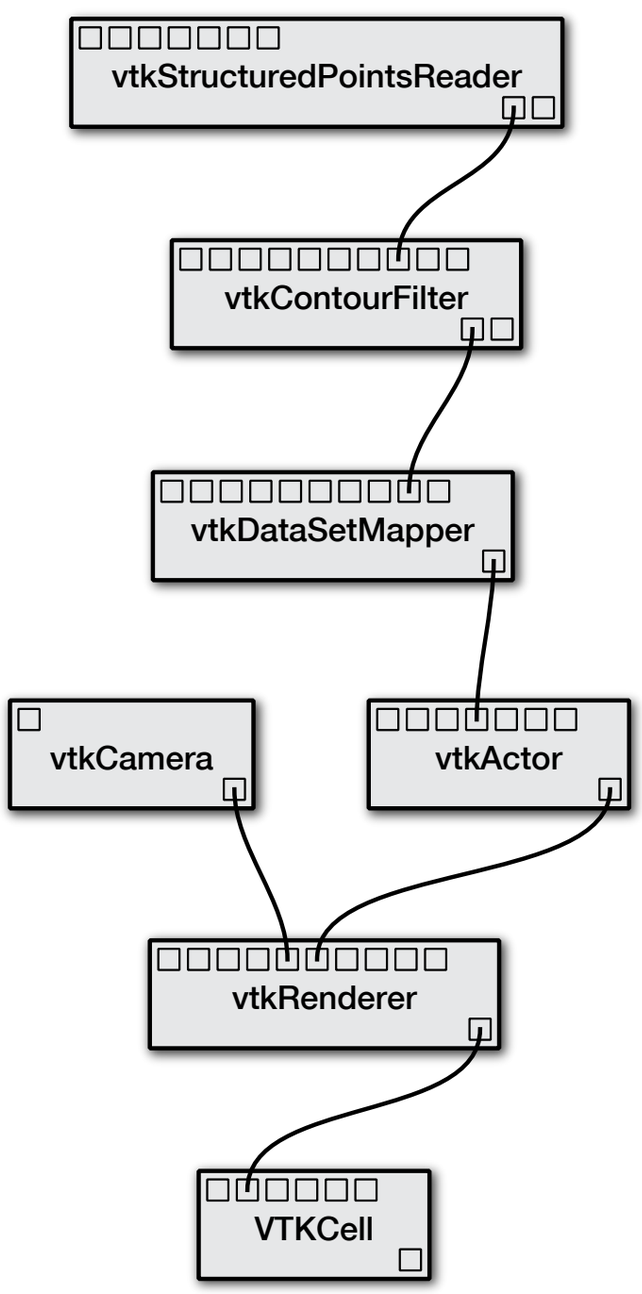
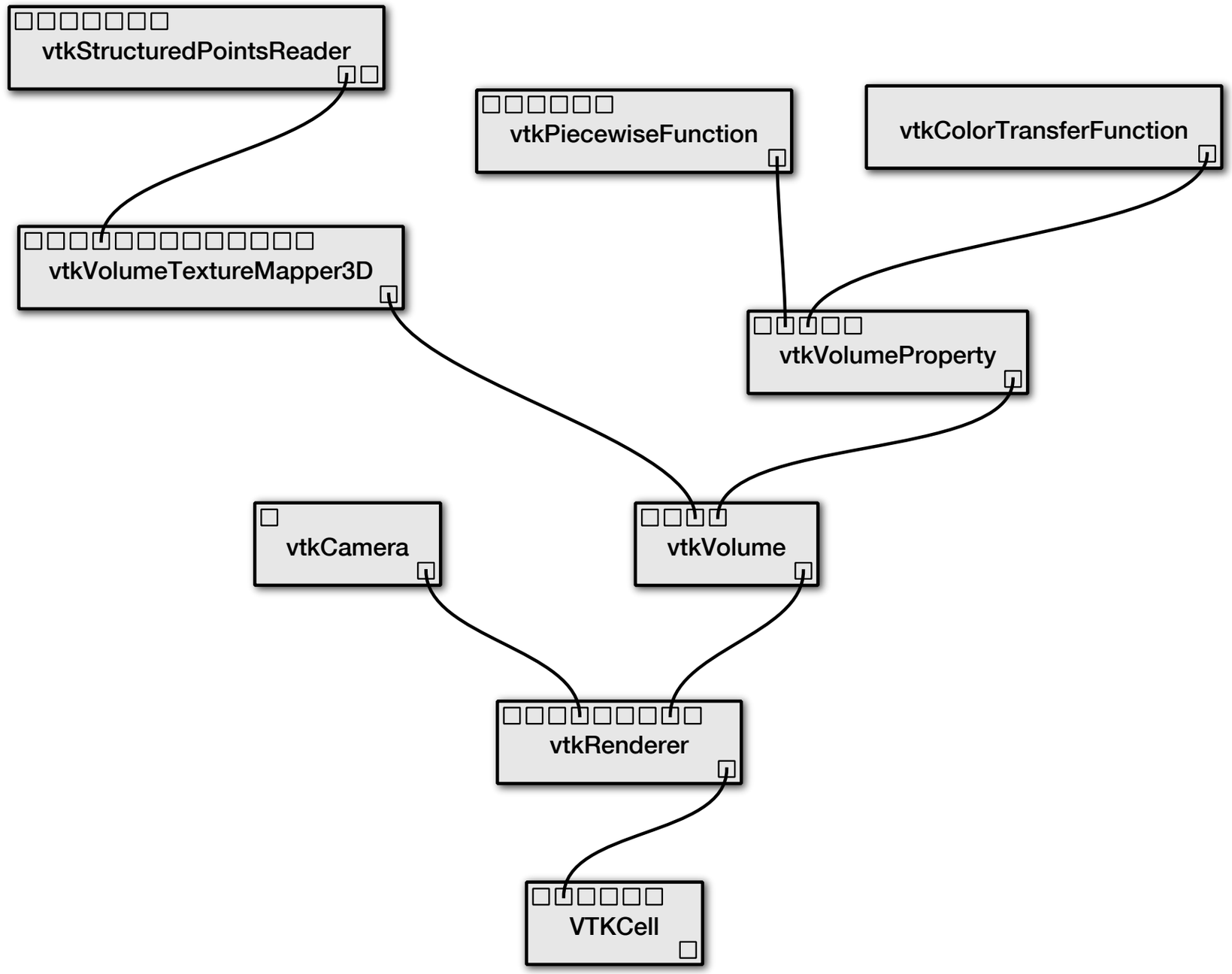


Workflow Differences





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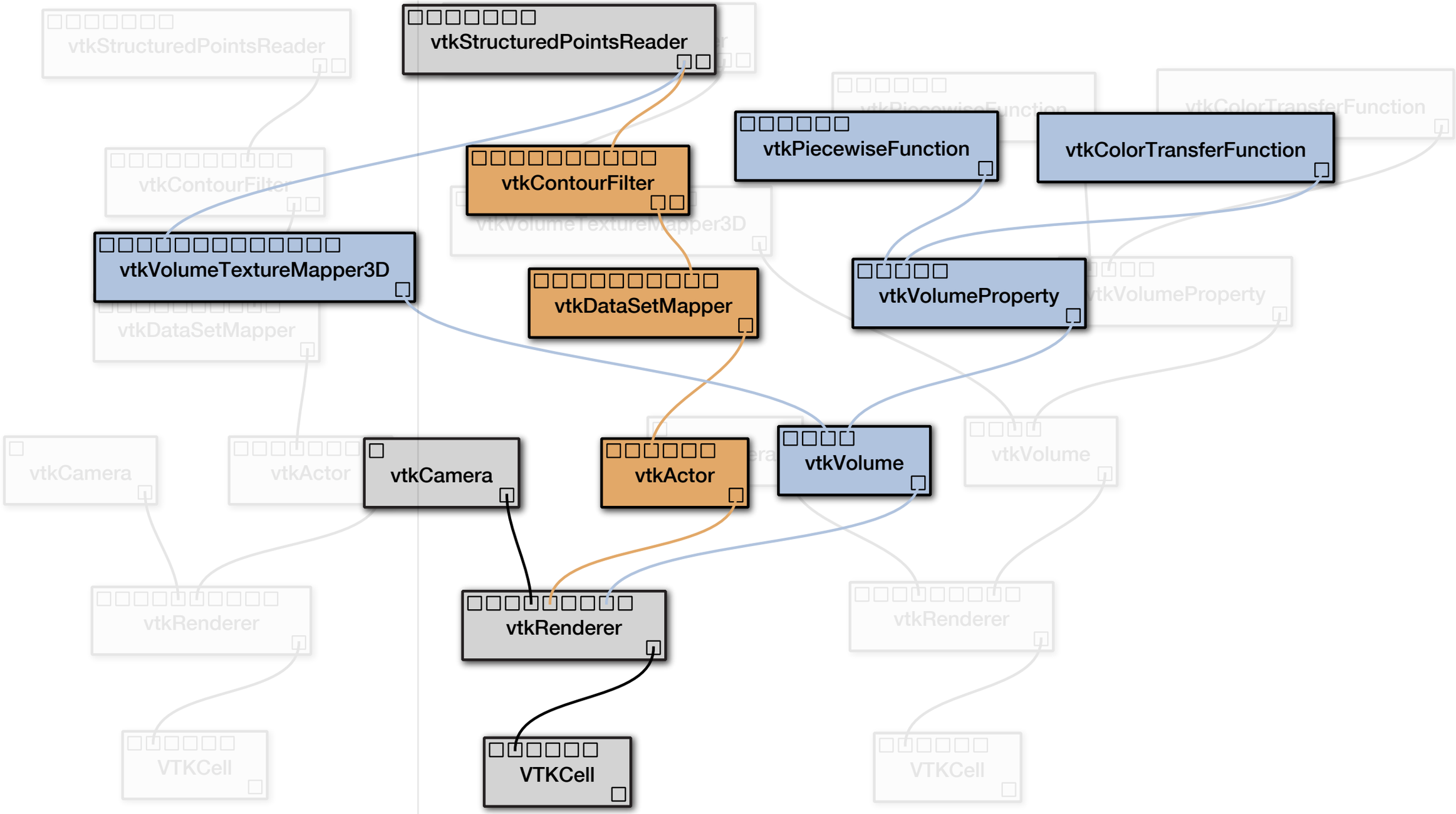
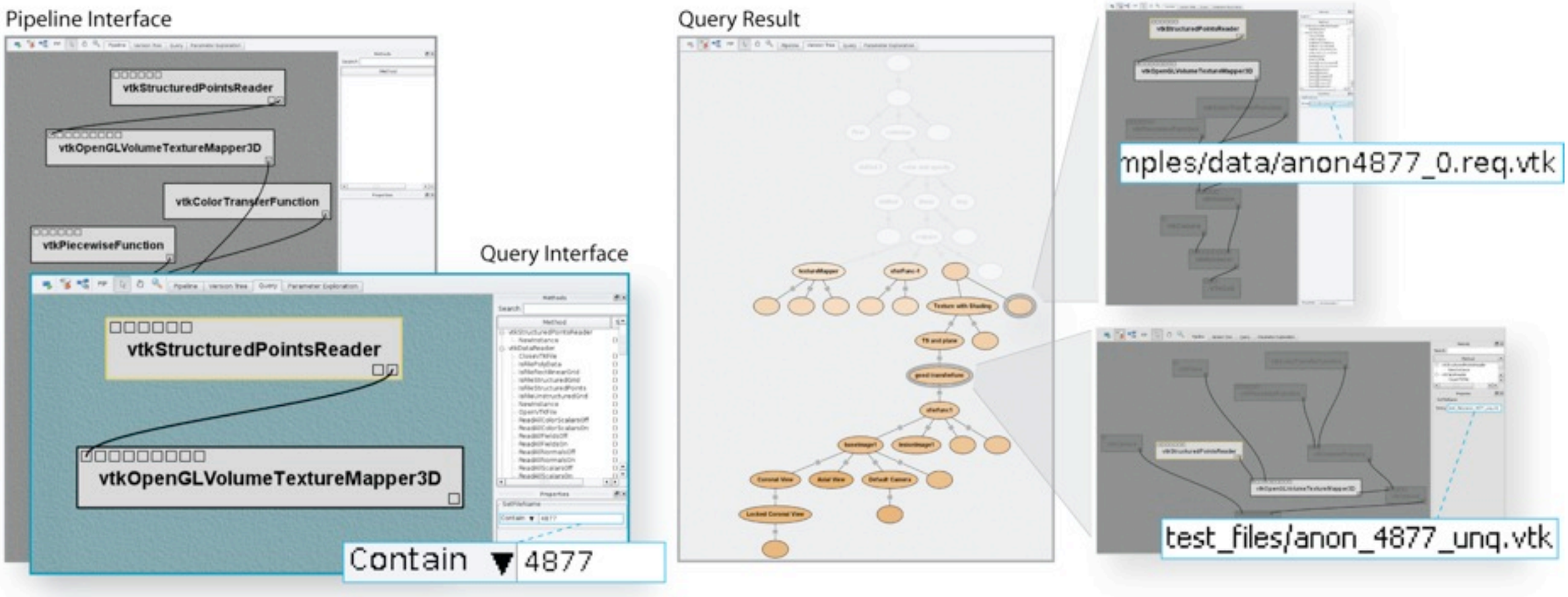
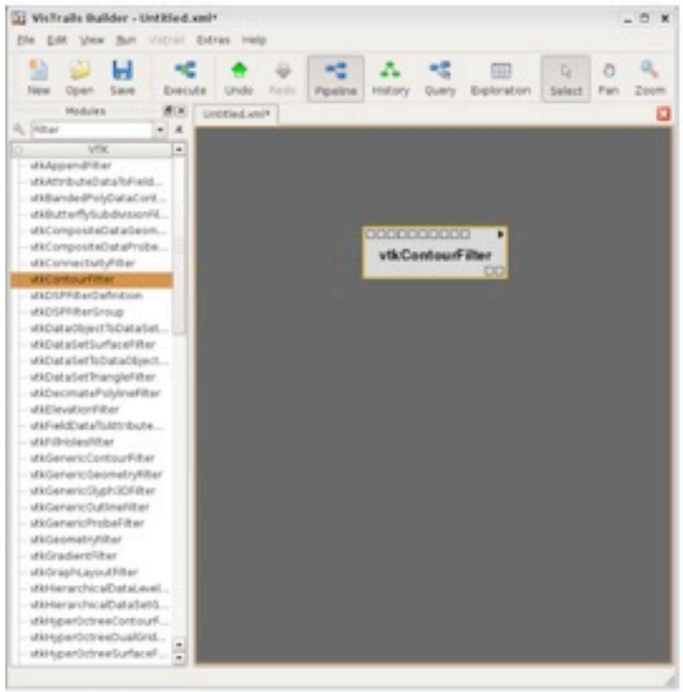


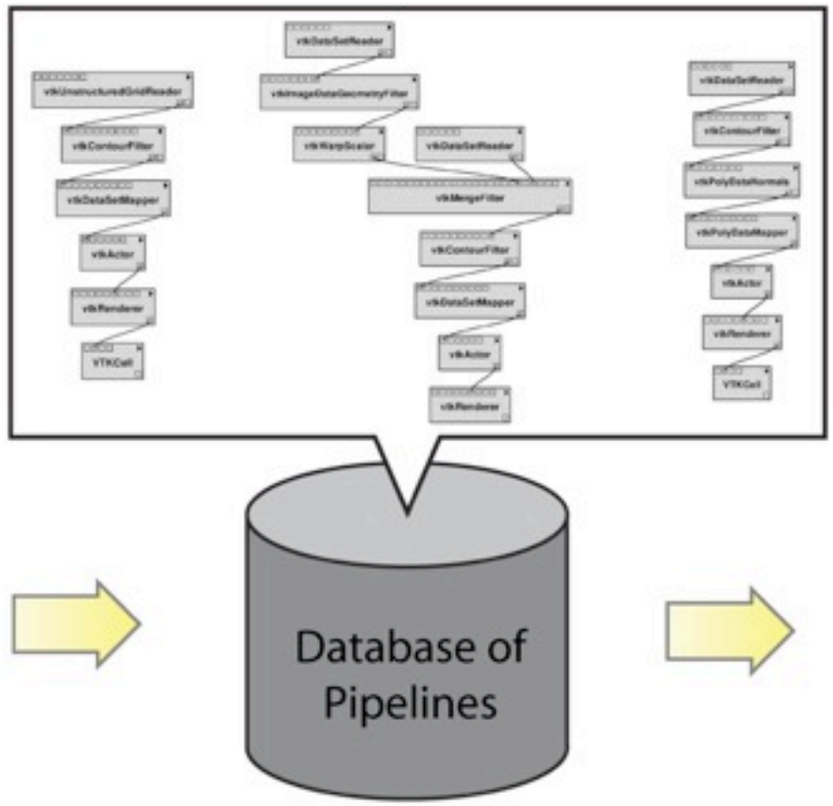
Workflow Query-by-example

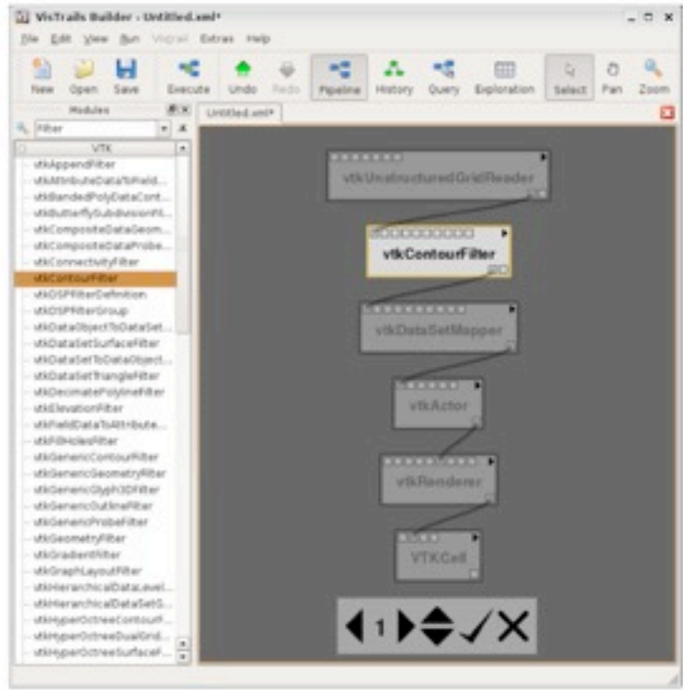


[IEEE Visualization 2007]

Workflow Completions







[IEEE Visualization 2008]

Provenance in Art

Rembrandt van Rijn
Dutch, 1606 - 1669
***Self-Portrait*, 1659**
oil on canvas
Andrew W. Mellon Collection
1937.1.72

Provenance

George, 3rd Duke of Montagu and 4th Earl of Cardigan [d. 1790], by 1767;[1] by inheritance to his daughter, Lady Elizabeth, wife of Henry, 3rd Duke of Buccleuch of Montagu House, London; John Charles, 7th Duke of Buccleuch; (P. & D. Colnaghi & Co., New York, 1928); (M. Knoedler & Co., New York); sold January 1929 to Andrew W. Mellon, Pittsburgh and Washington, D.C.; deeded 28 December 1934 to The A.W. Mellon Educational and Charitable Trust, Pittsburgh; gift 1937 to NGA.

[1] This early provenance is established by presence of a mezzotint after the portrait by R. Earlom (1743-1822), dated 1767. See John Charrington, *A Catalogue of the Mezzotints After, or Said to Be After, Rembrandt*, Cambridge, 1923, no. 49.

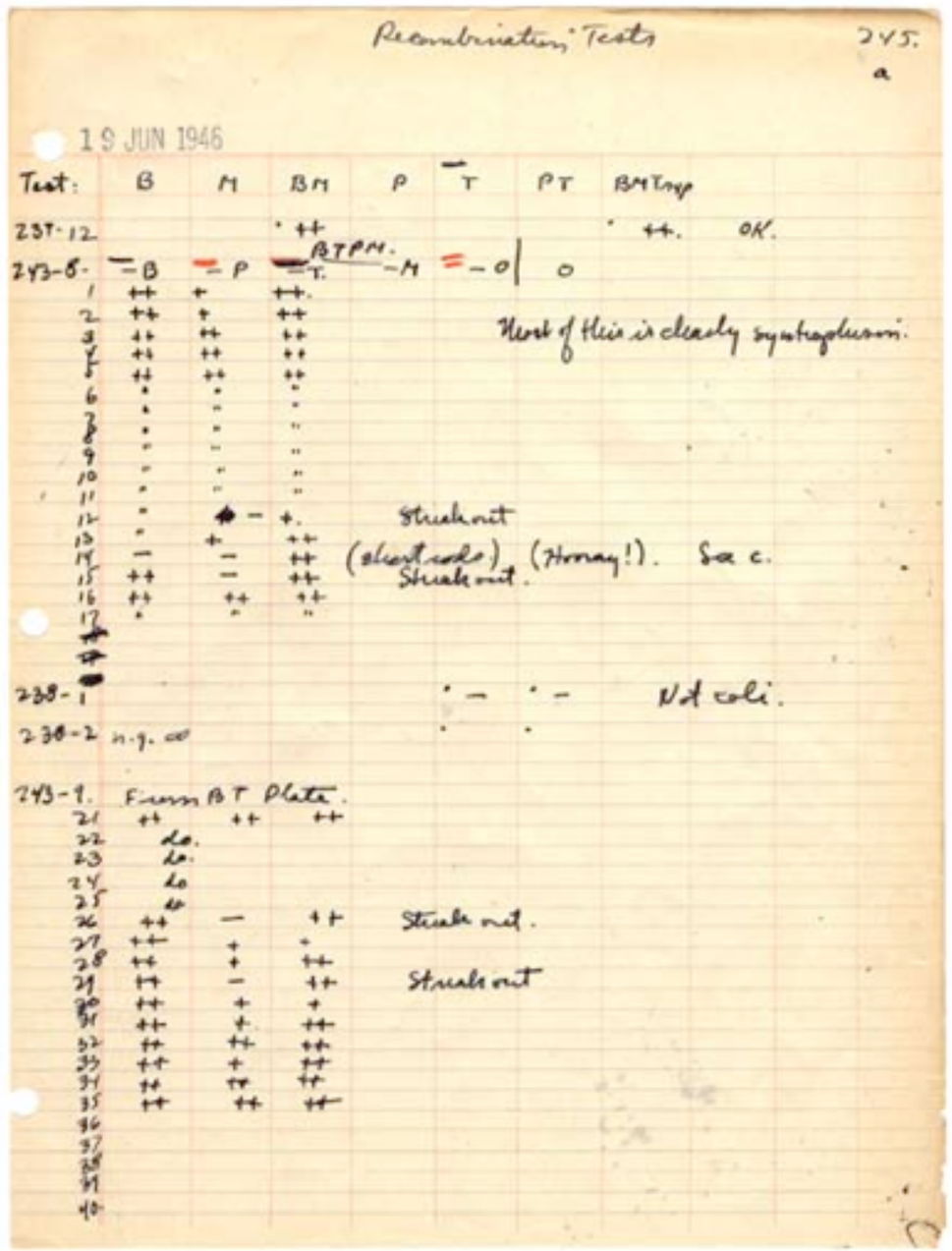
Associated Names

- Buccleuch, Henry, 3rd Duke of
- Buccleuch, John Charles, 7th Duke of
- Colnaghi & Co., Ltd., P. & D.
- Knoedler & Company, M.
- Mellon, Andrew W.
- Mellon Educational and Charitable Trust, The A.W.
- Montagu, and 4th Earl of Cardigan, George, 3rd Duke of

[National Gallery of Art]

Provenance in Science

- **Provenance is as (or more) important as the result!**
- Old solution:
  - Lab notebooks
- New problems:
  - Large volumes of data
  - Complex analyses
  - Writing notes doesn't scale
- New solution:
  - Automated provenance capture with user-defined annotations



[DNA Recombination, Lederberg]

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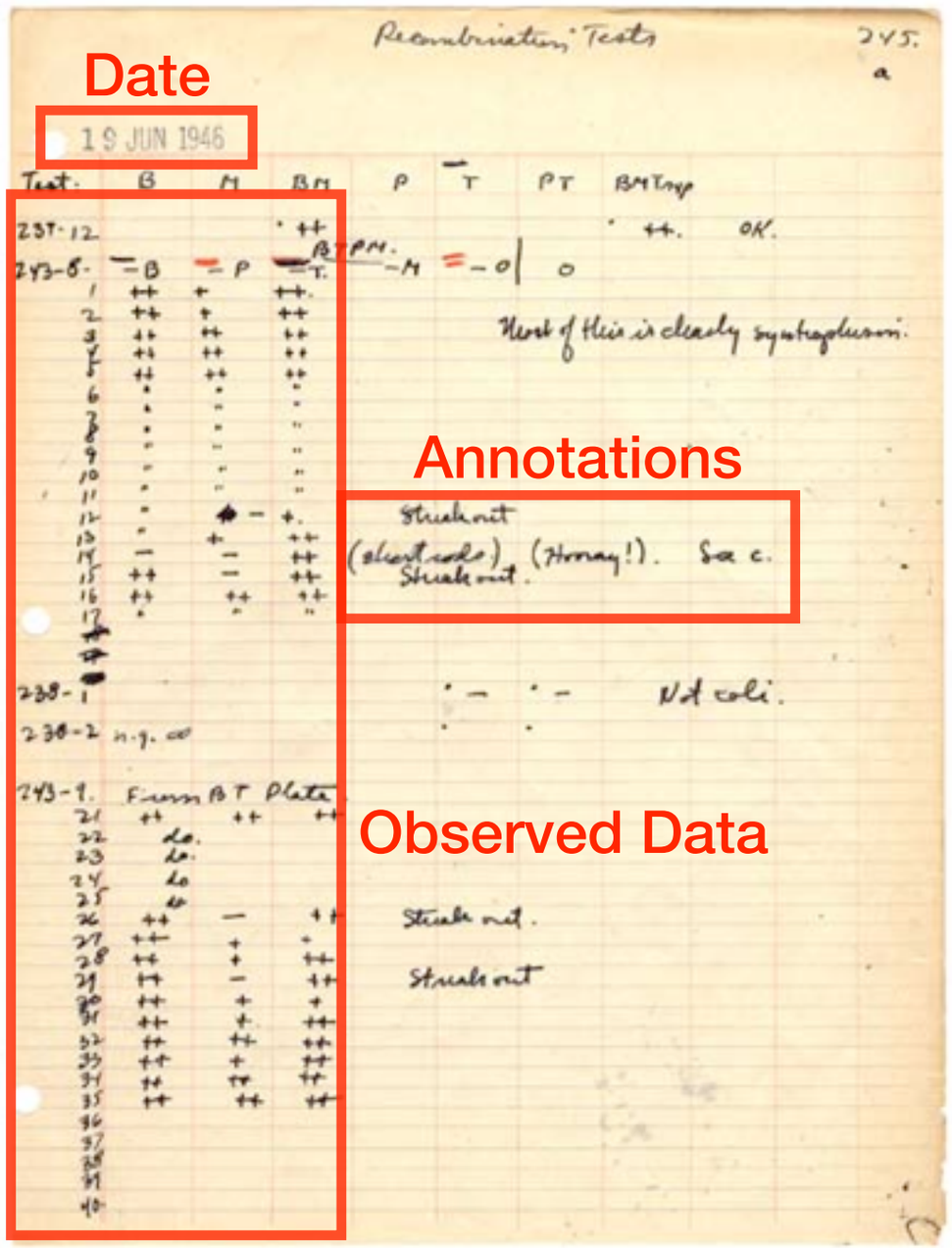
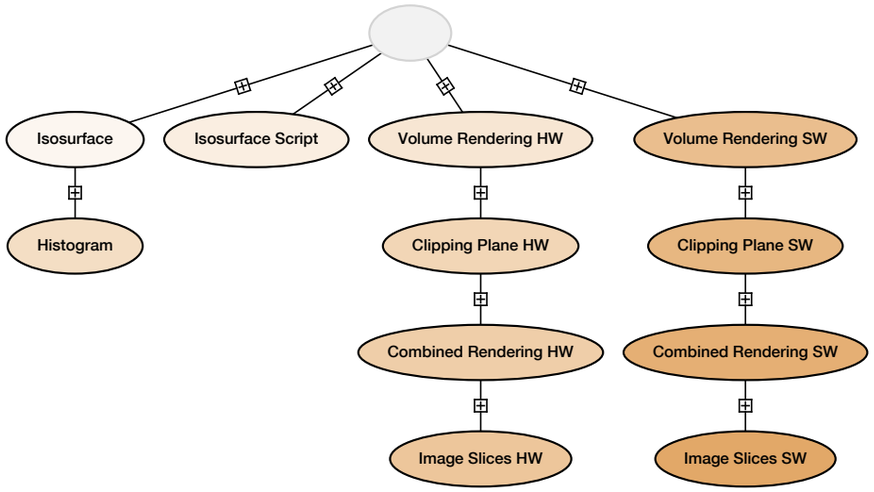


[DNA Recombination, Lederberg]

Provenance in VisTrails

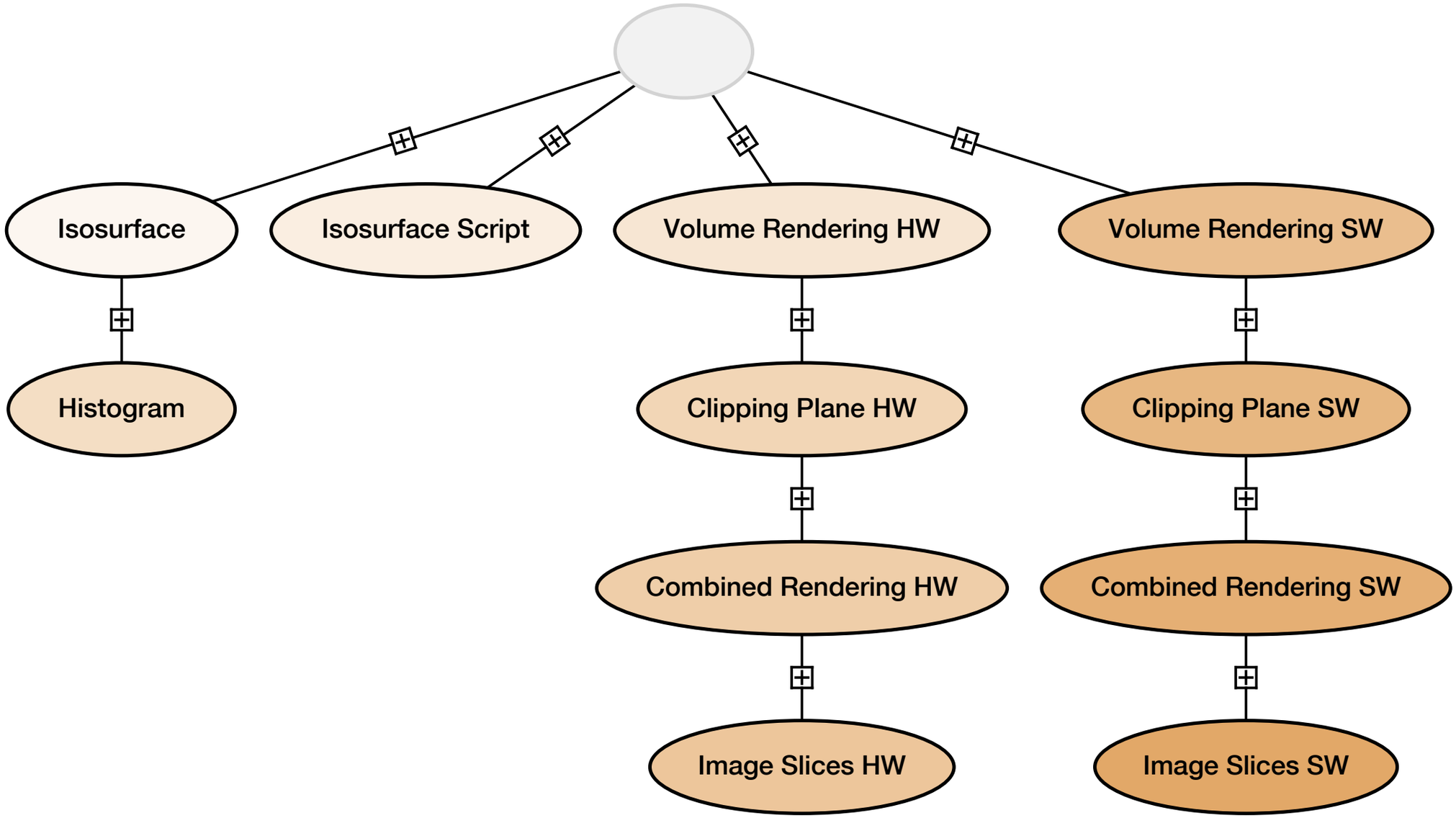
- Design Provenance (Version Tree)



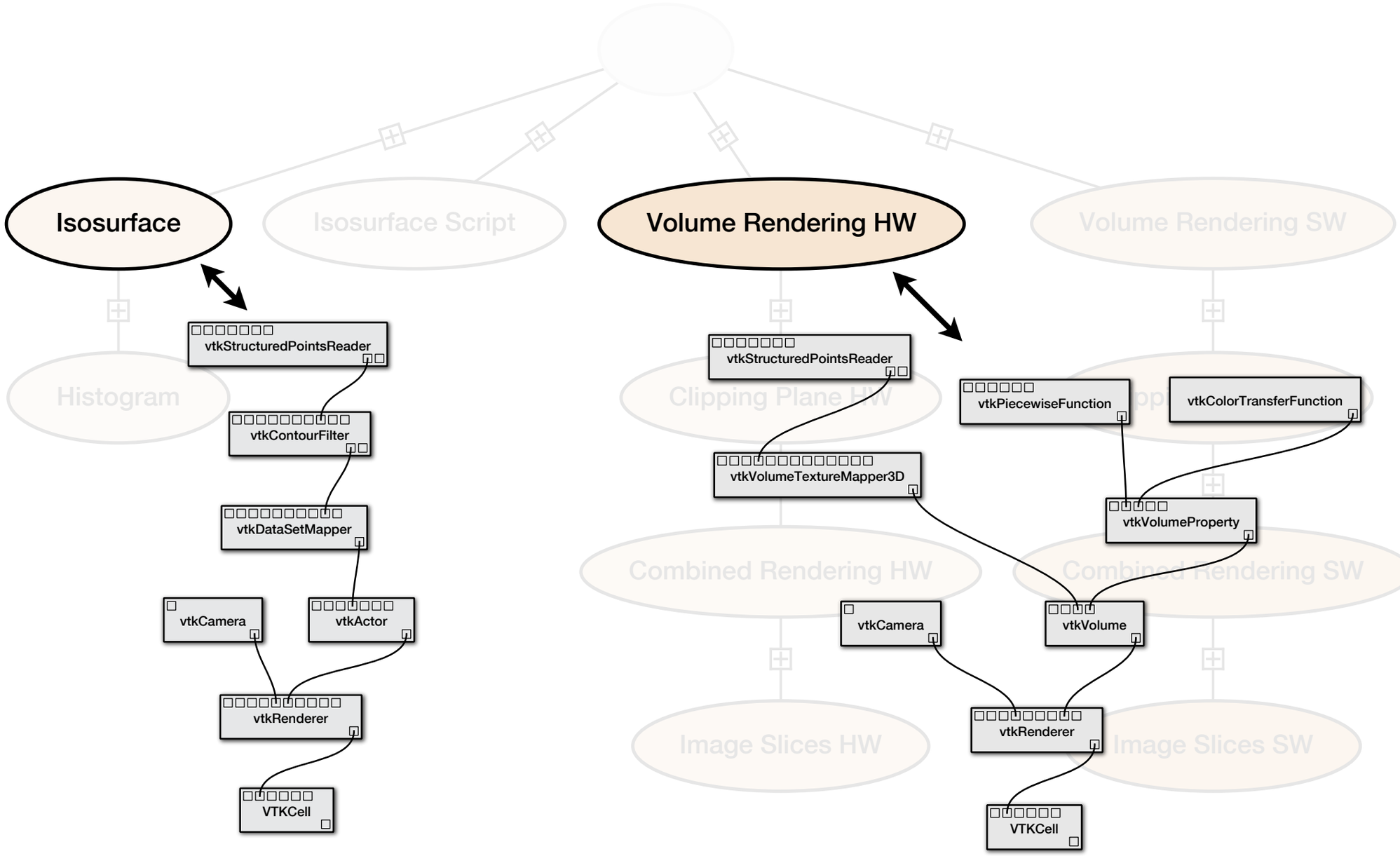
- Execution Provenance (Logging):

```
<module id="12" name="vtkDataSetReader" start_time="2010-02-19 11:01:05"
     end_time="2010-02-19 11:01:07">
  <annotation key="hash" value="c54bea63cb7d912a43ce"/>
</module>
<module id="13" name="vtkContourFilter" start_time="2010-02-19 11:01:07"
     end_time="2010-02-19 11:01:08"/>
<module id="15" name="vtkDataSetMapper" start_time="2010-02-19 11:01:09"
     end_time="2010-02-19 11:01:12"/>
```

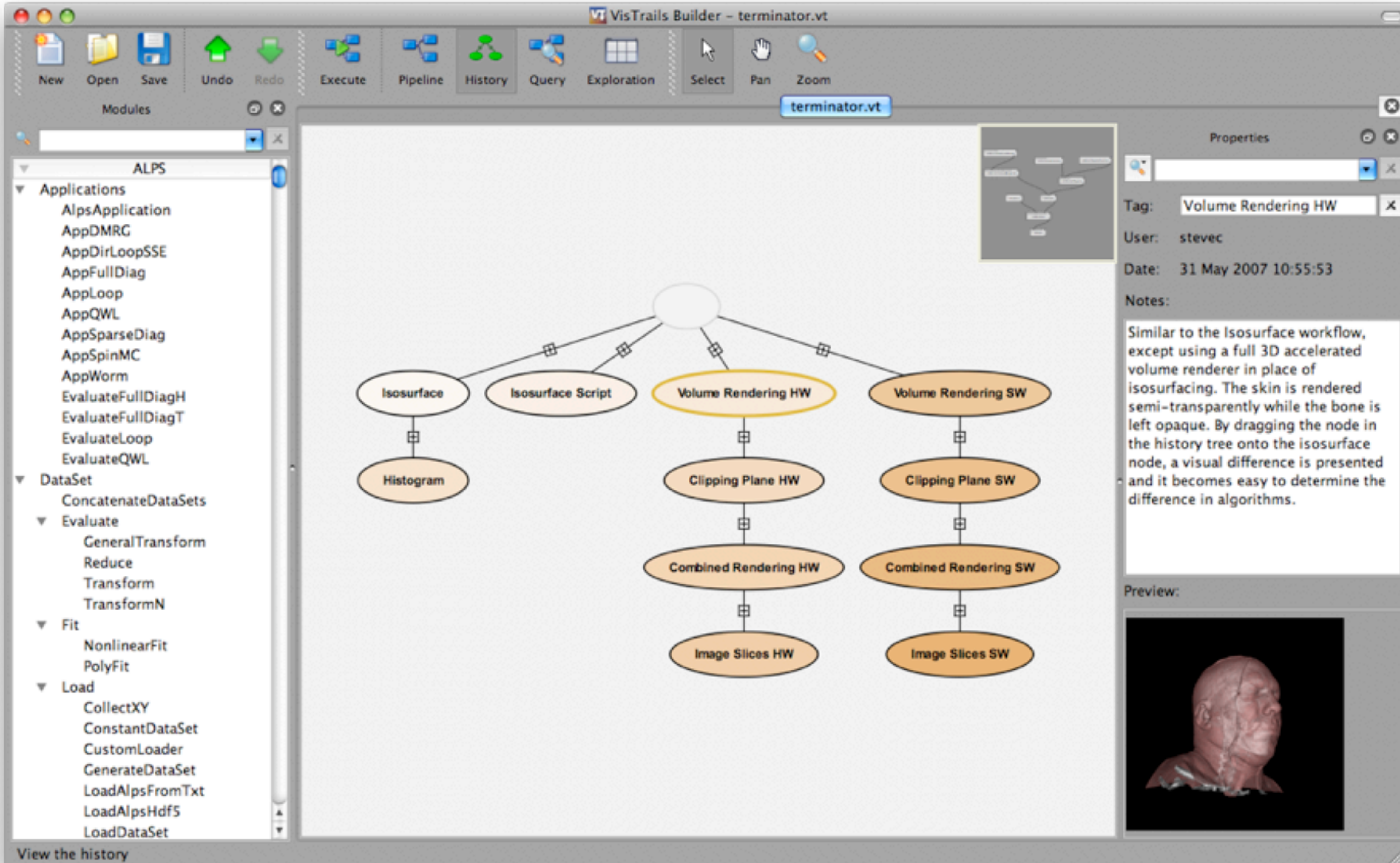
Design Provenance



Design Provenance



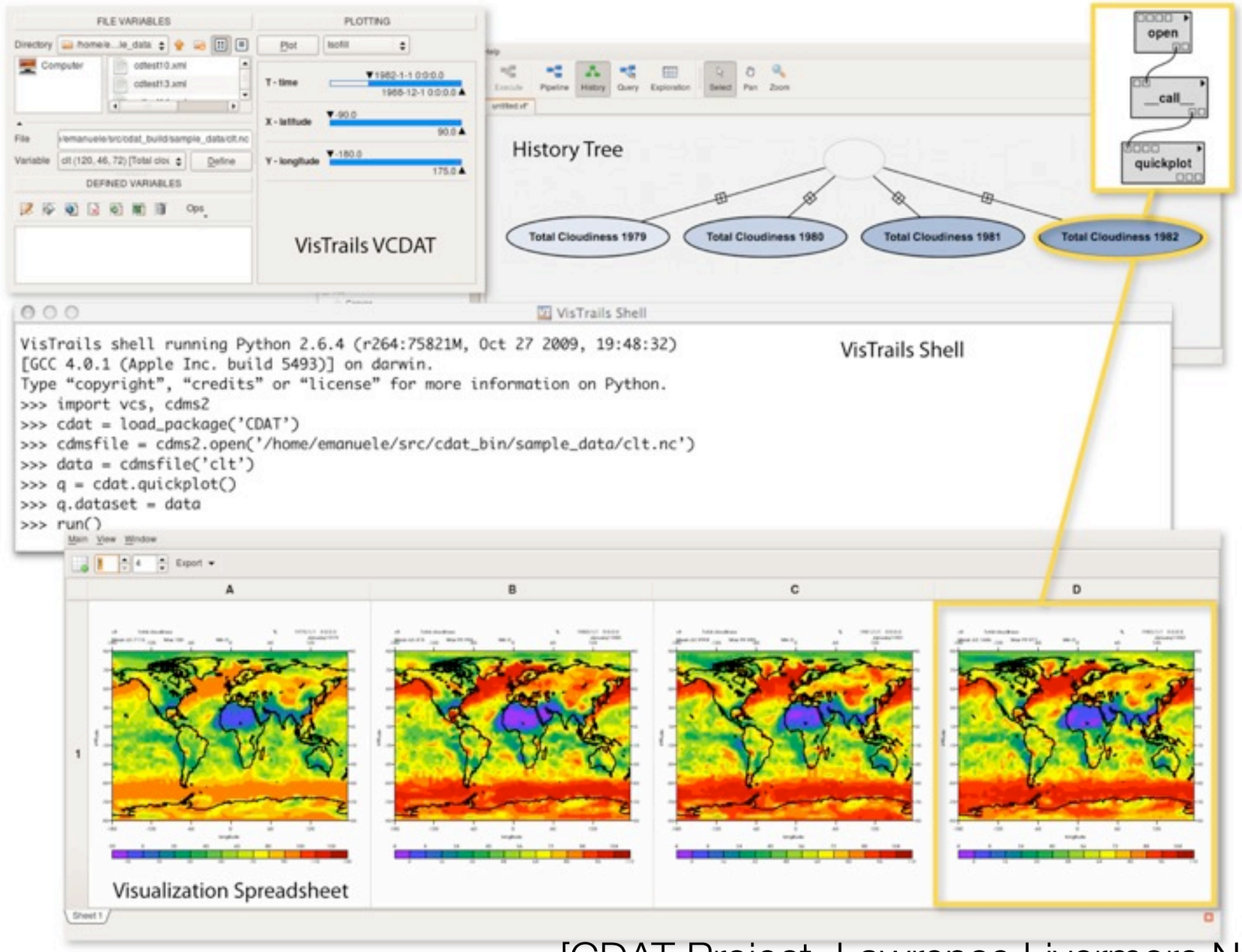
VisTrails - Design Provenance



Specifications

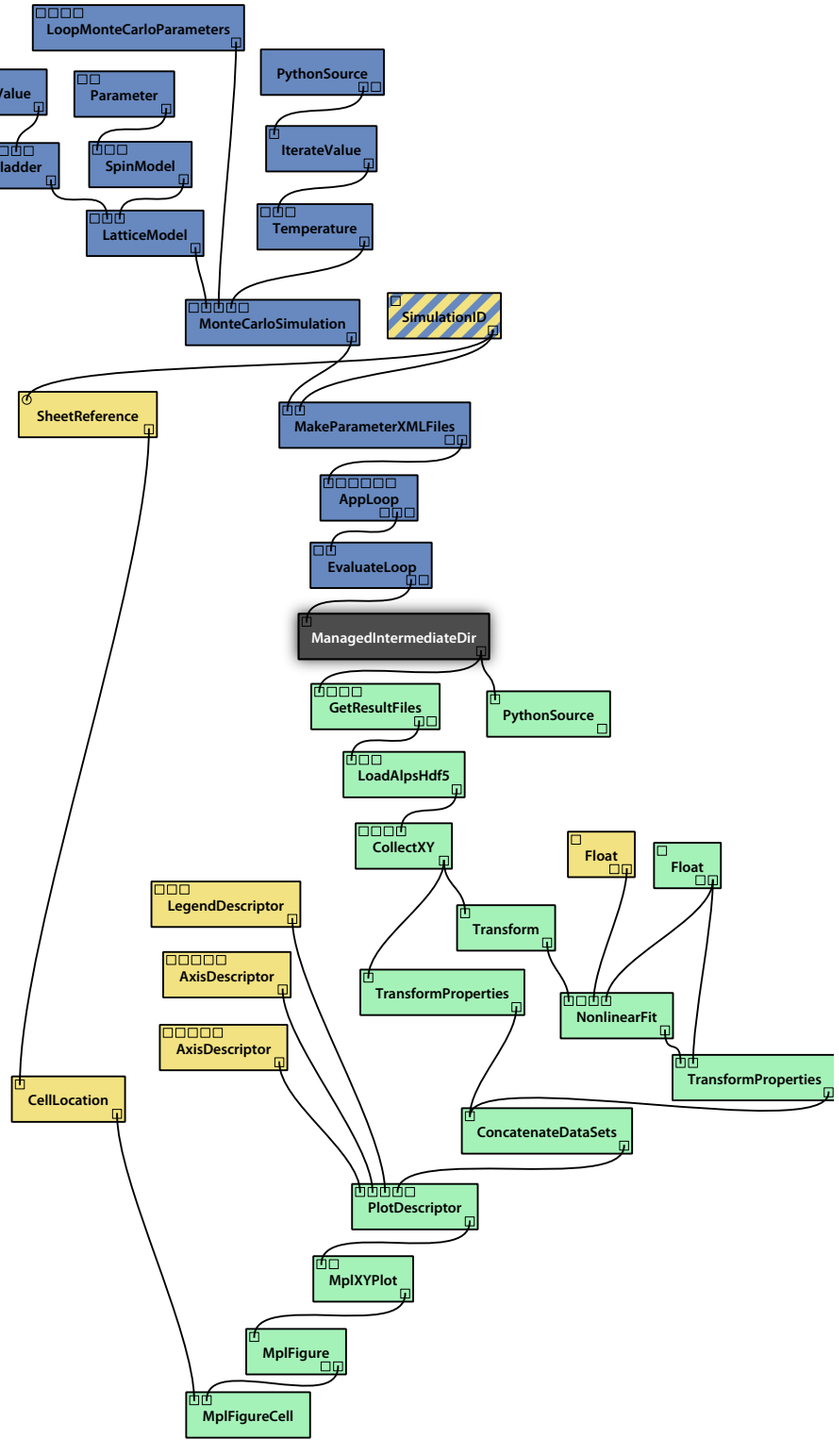
- Open-source, freely downloadable system (www.vistrails.org)
- Multi-platform: users on Mac, Linux, and Windows
- Python code and uses PyQt and Qt for the interface
- Over 13,000 downloads since 2007
- User's guide, wiki, and mailing list
- Many users in different disciplines and countries:
  - Visualizing environmental simulations (CMOP STC)
  - Simulation for solid, fluid and structural mechanics (Galileo Network, UFRJ Brazil)
  - Quantum physics simulations (ALPS, ETH Switzerland)
  - Climate analysis (CDAT)
  - Habitat modeling (USGS)
  - Open Wildland Fire Modeling (U. Colorado, NCAR)
  - High-energy physics (LEPP, Cornell)
  - Cosmology simulations (LANL)
  - Using tms for improving memory (Pyschiatry, U. Utah)
  - eBird (Cornell, NSF DataONE)
  - Astrophysical Systems (Tohline, LSU)
  - NIH NBCR (UCSD)
  - Pervasive Technology Labs (Heiland, Indiana University)
  - Linköping University
  - University of North Carolina, Chapel Hill
  - UTEP

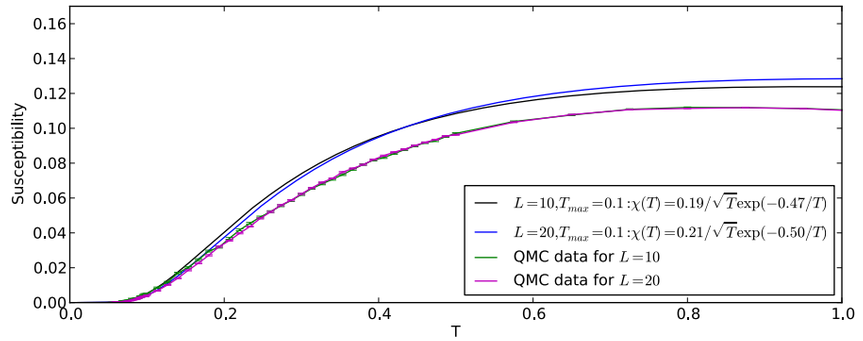
Climate Data Analysis

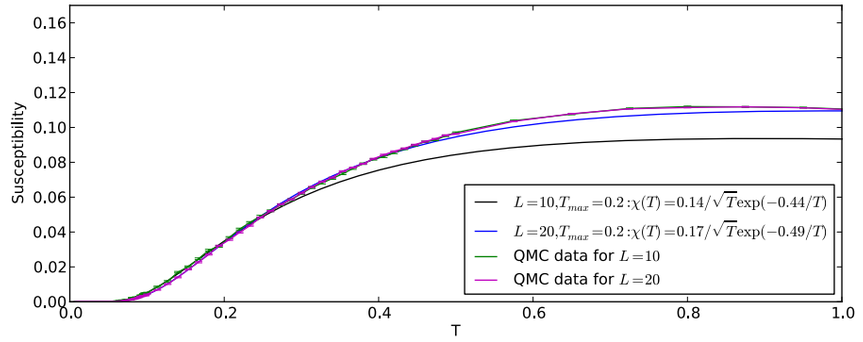


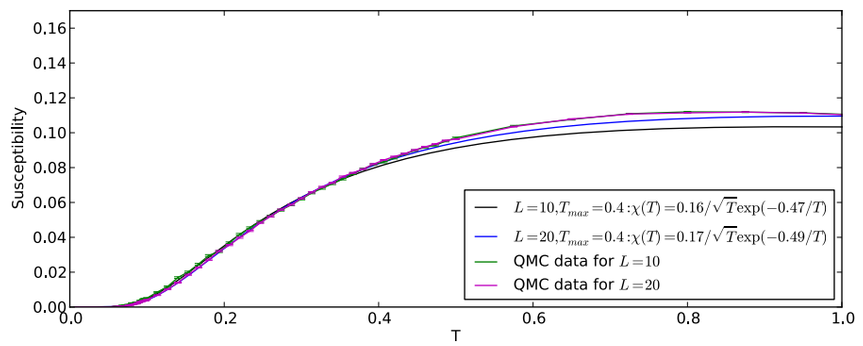
[CDAT Project, Lawrence Livermore National Lab]

Quantum Lattice Models



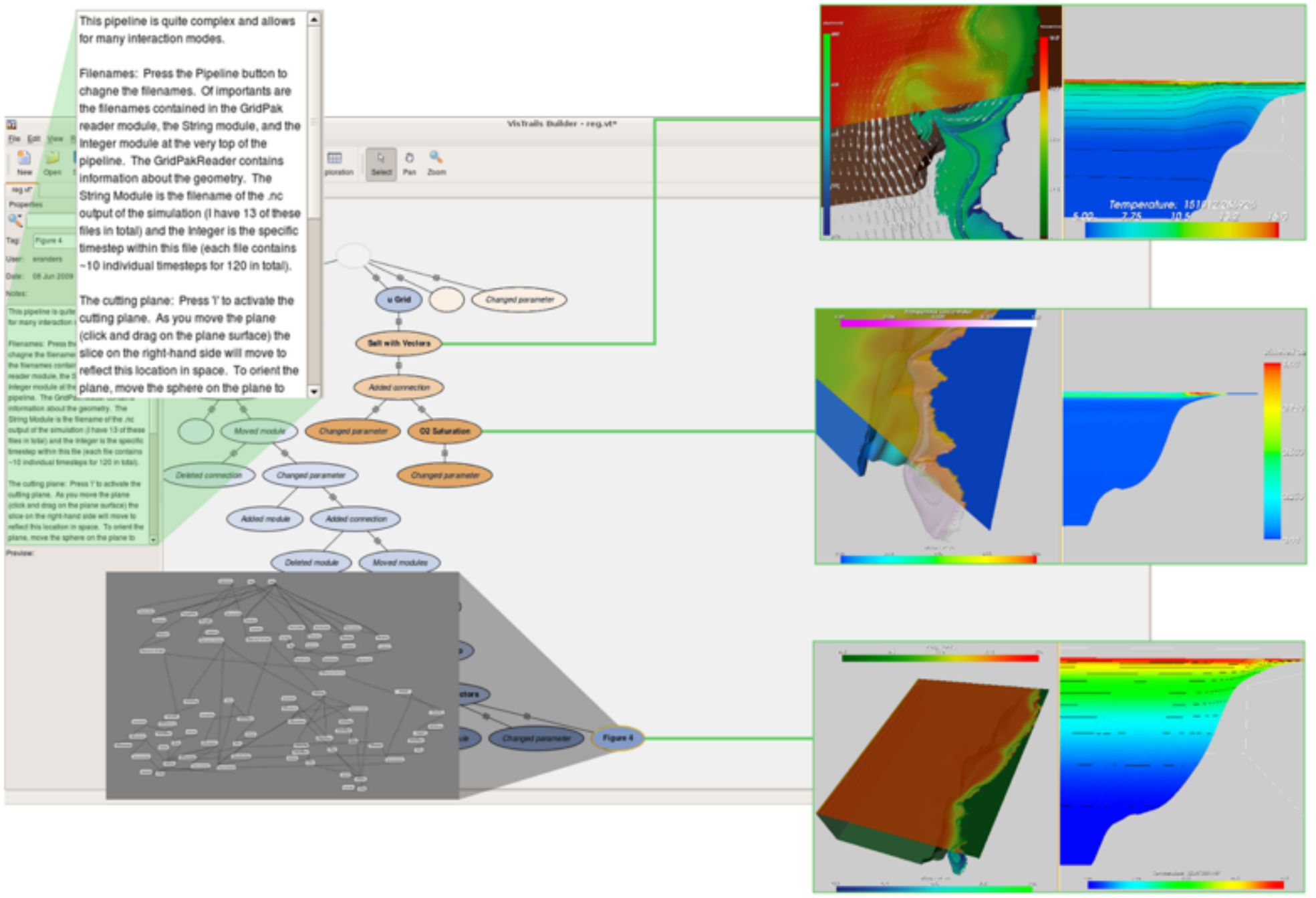






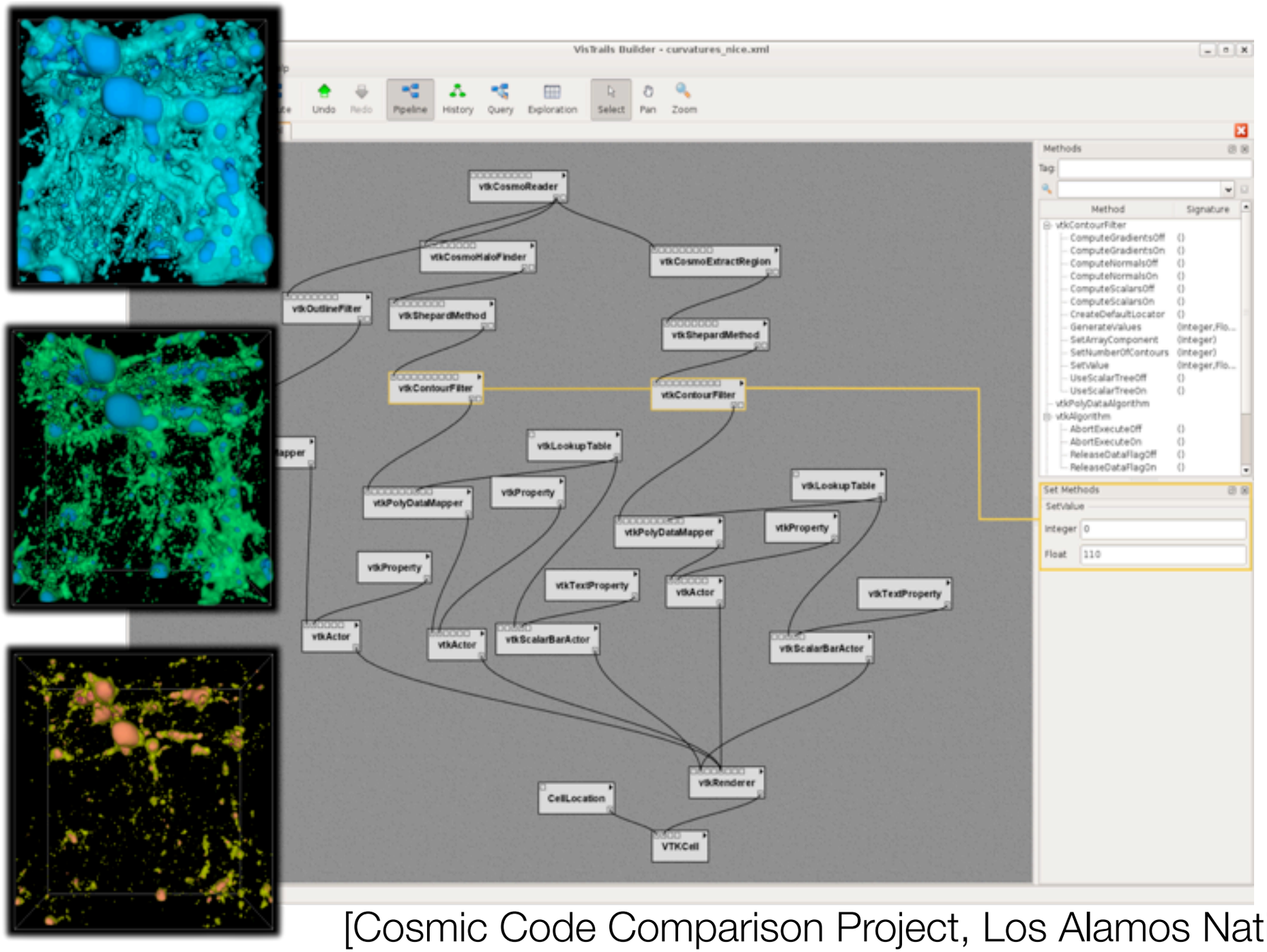
[ALPS Project, ETH-Zurich]

Coastal Margin Observation & Prediction



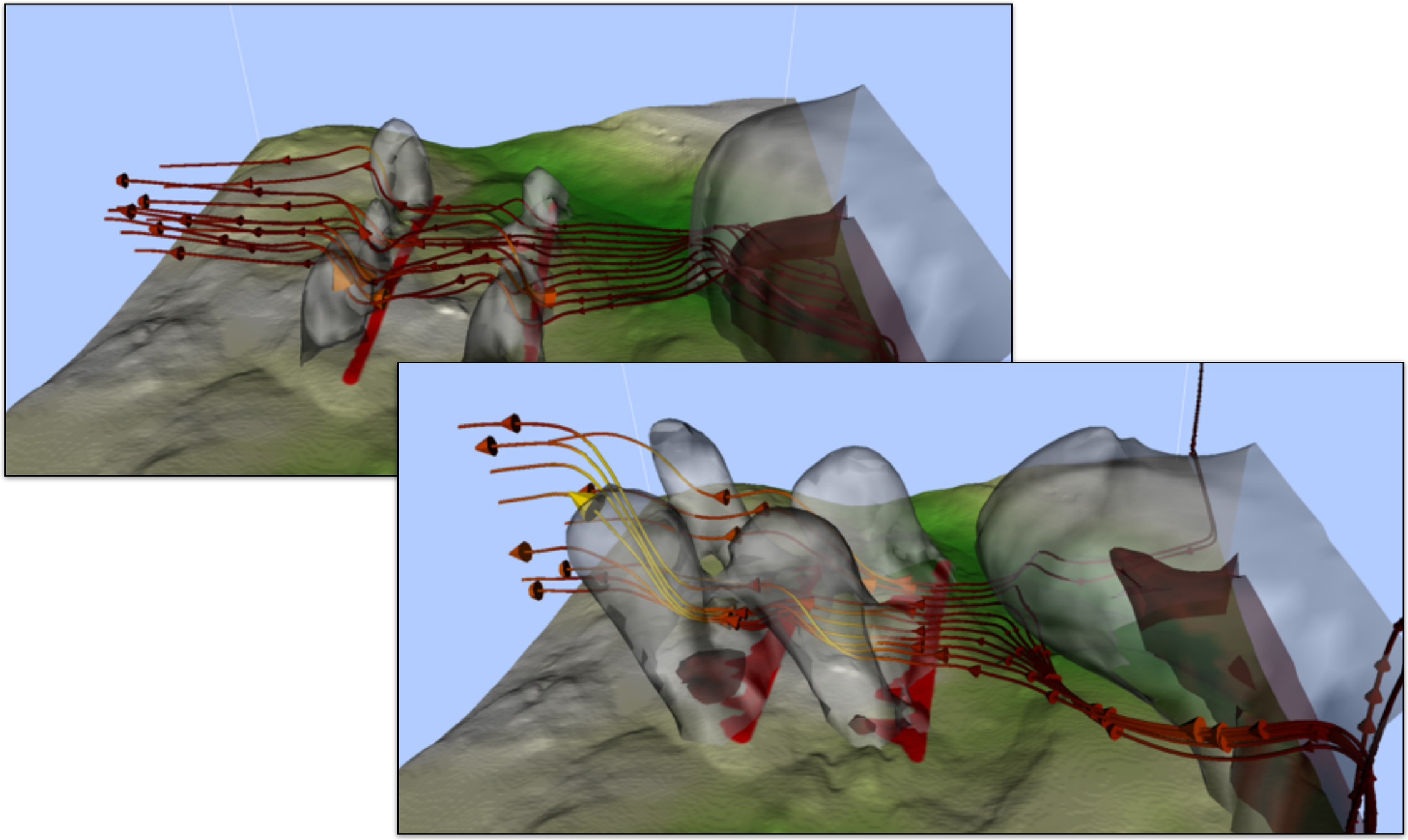
[NSF Science & Technology Center for Coastal Margin Observation & Prediction]

Comparing Cosmological Simulations



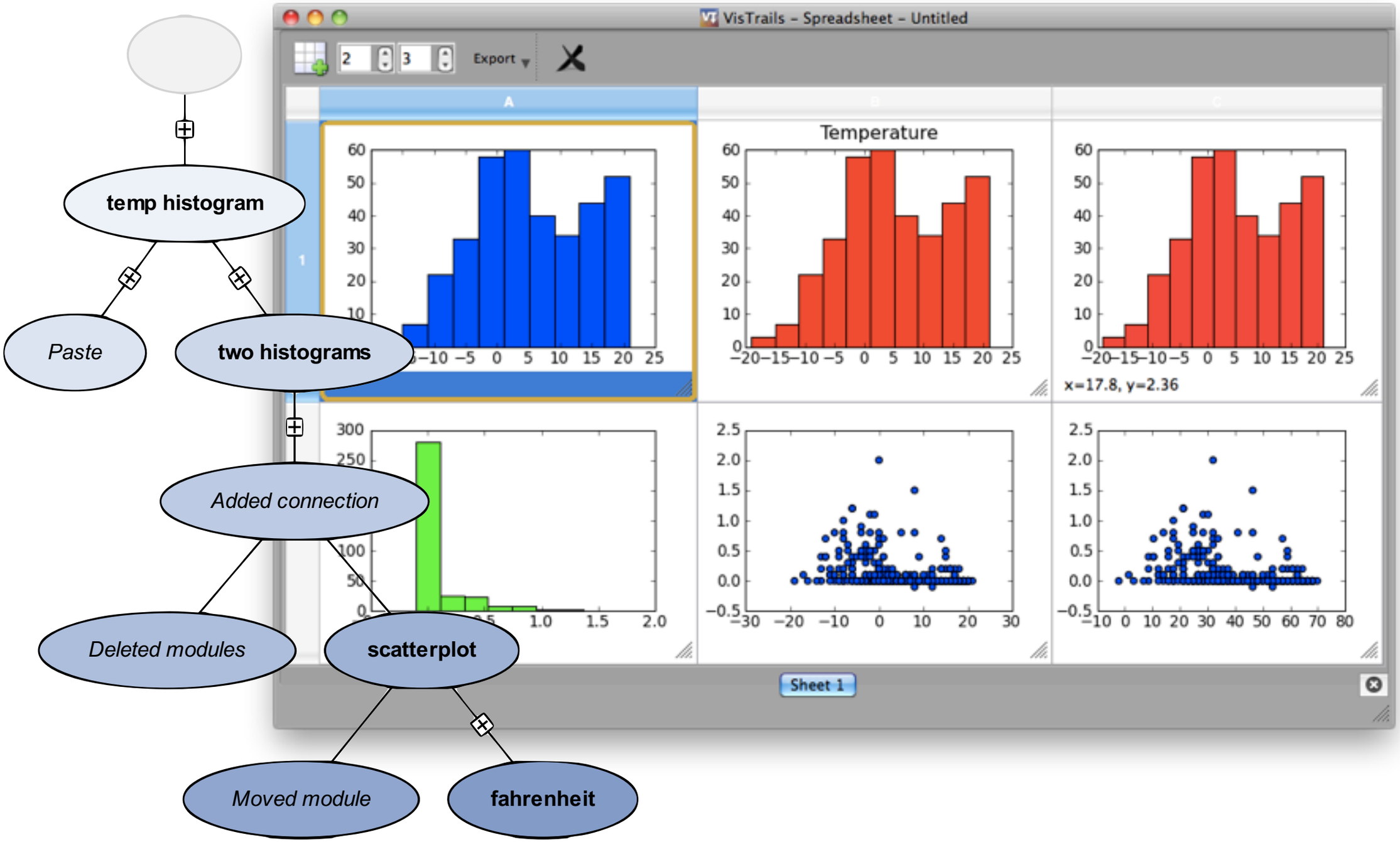
[Cosmic Code Comparison Project, Los Alamos National Lab]

Wildfire Prediction



[WRF-Fire Project, University of Colorado-Denver]

Demo


VisTrails - Spreadsheet - Untitled
Export
Temperature
x=17.8, y=2.36
Sheet 1
temp histogram
Paste
two histograms
Added connection
Deleted modules
scatterplot
Moved module
fahrenheit

Extensibility

- Package infrastructure
- Wrap python libraries, command-line calls, or use other interfaces (jpype, rpy, etc.)
- Need to specify:
  1. Package identification information
  2. Module structures: input & output ports
  3. Compute method for each module

Extensibility Example

- seawater python package:
  - http://pypi.python.org/pypi/seawater/1.0.3

```
identifier = 'org.ocefpaf.seawater'
version = '1.0.3'
name = 'Seawater Routines'

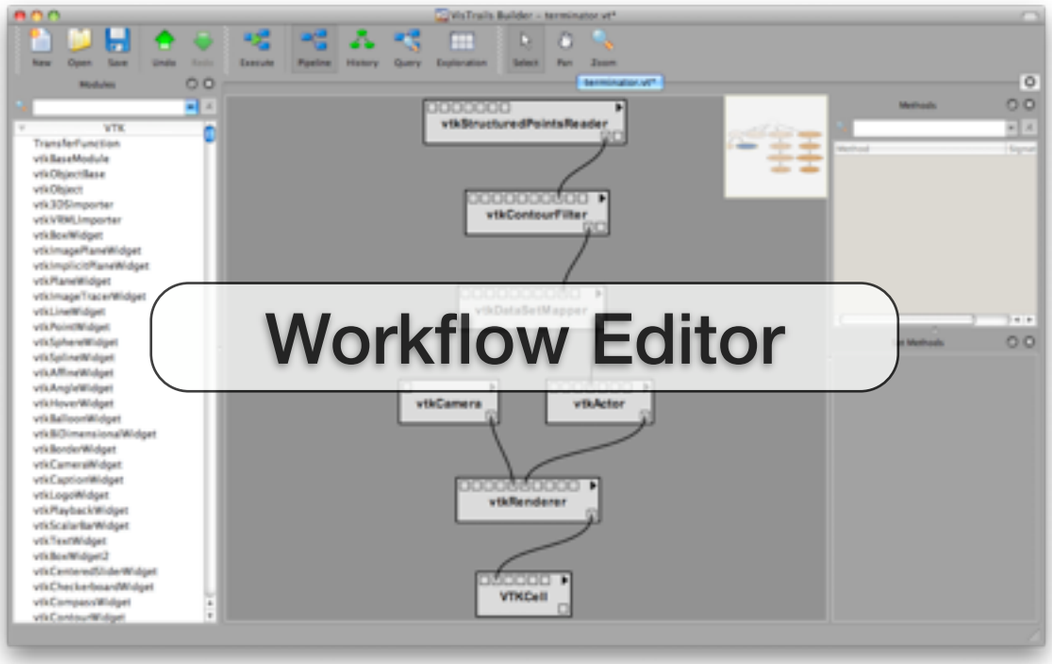
import seawater

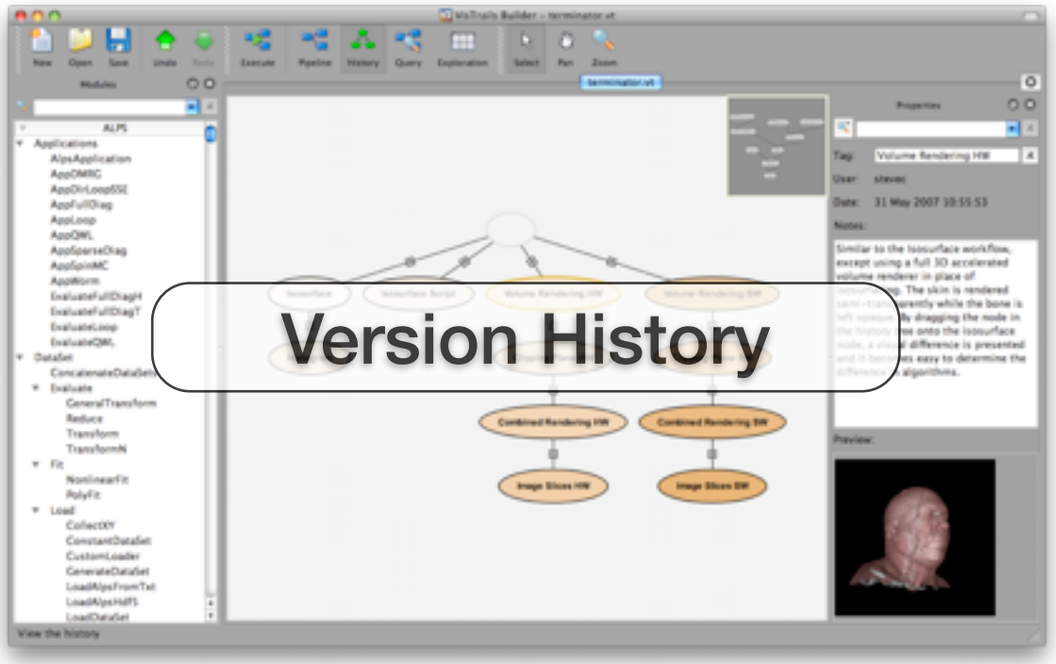
class SaturationN2(Module):
    _input_ports = [('S', Float),
                    ('T', Float)]
    _output_ports = [('res', Float)]

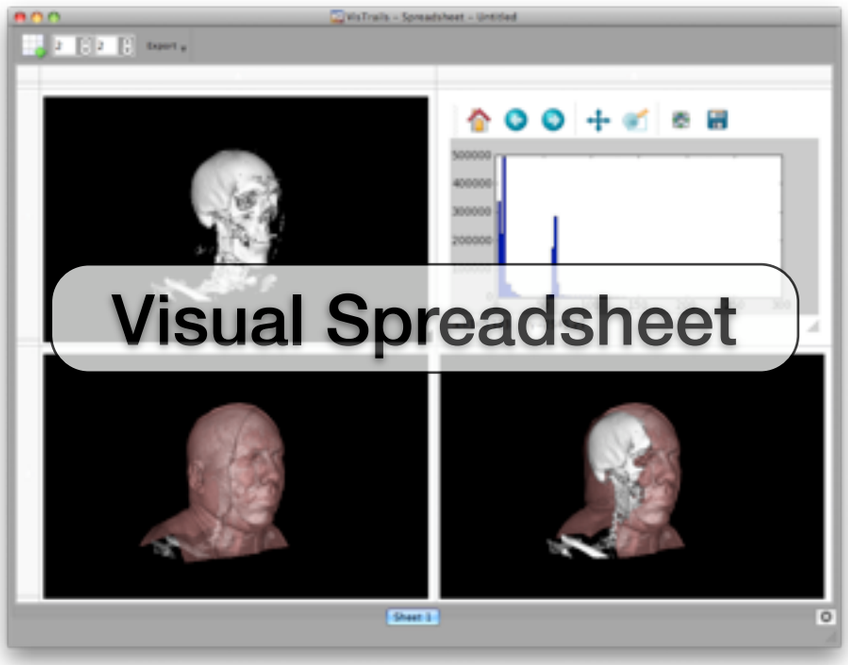
    def compute(self):
        s = self.getInputFromPort("S")
        t = self.getInputFromPort("T")
        res = seawater.satN2(s, t)
        self.setResult('res', res)

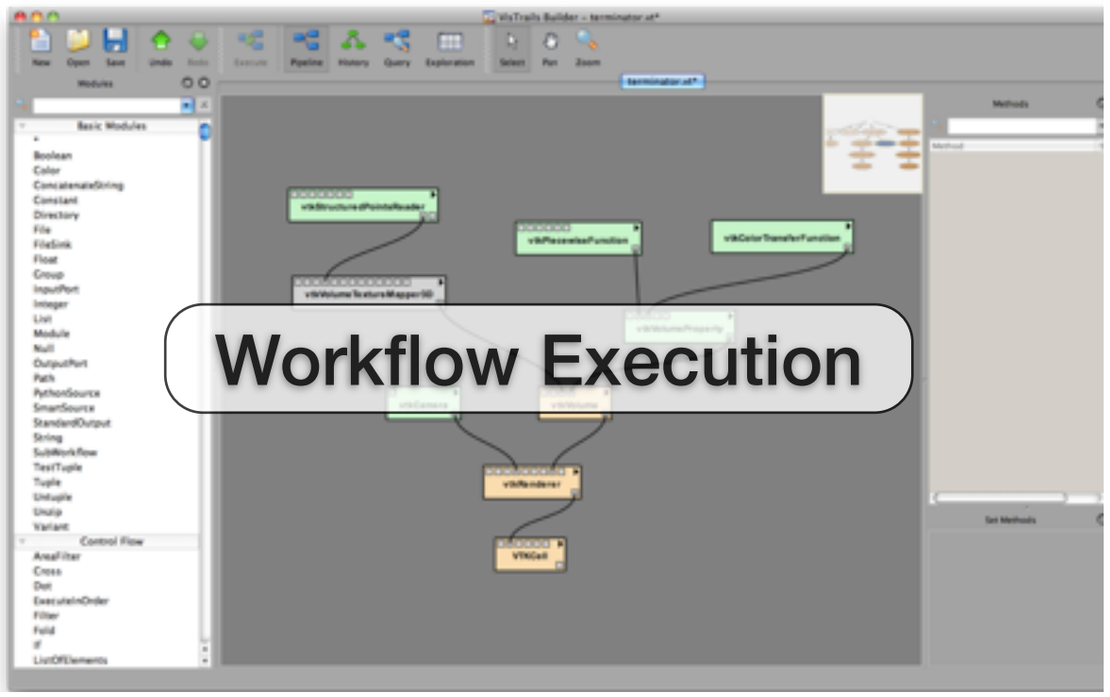
_modules = [SaturationN2,
```

VisTrails Components





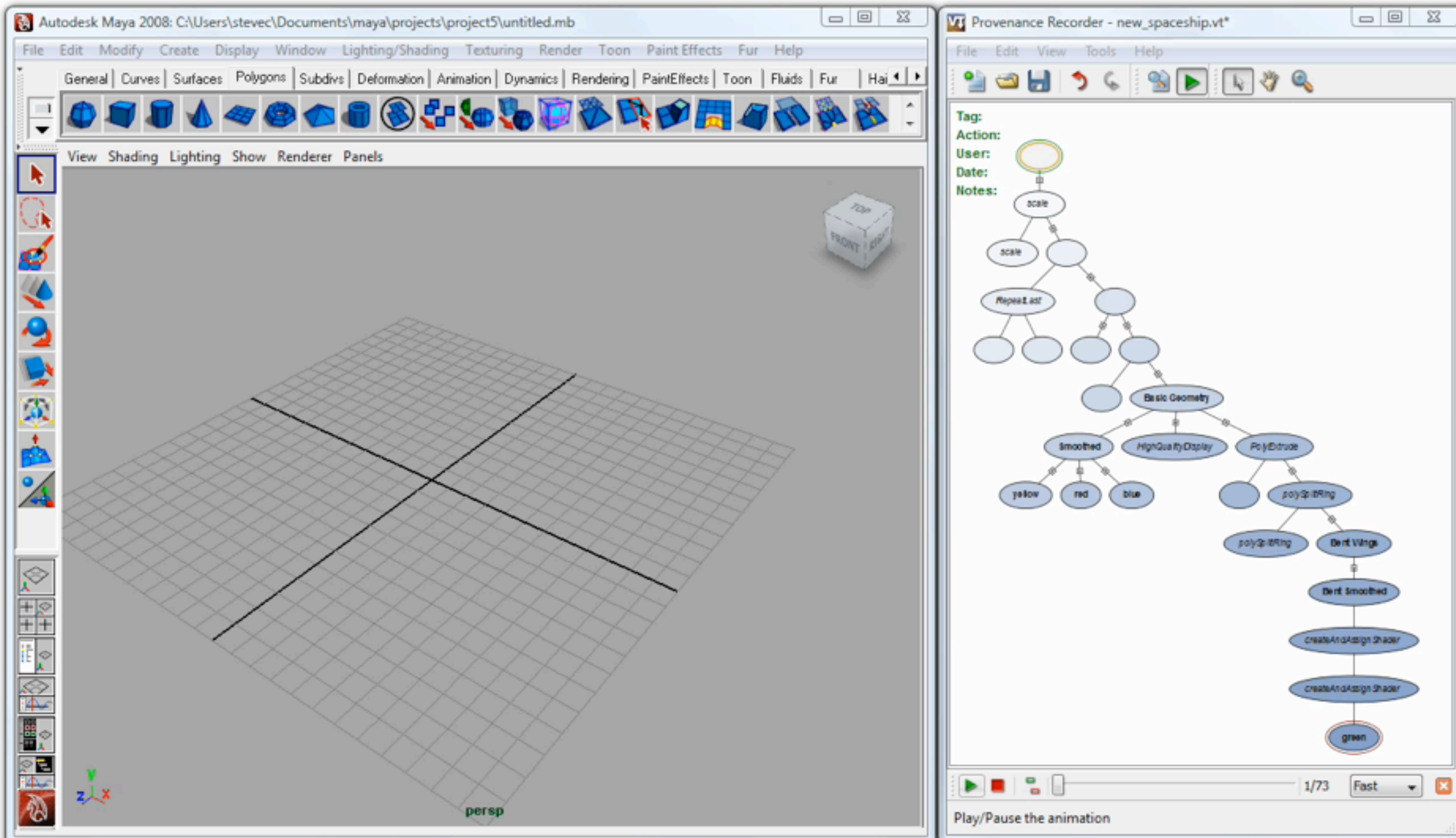




VisTrails Maya Plug-in

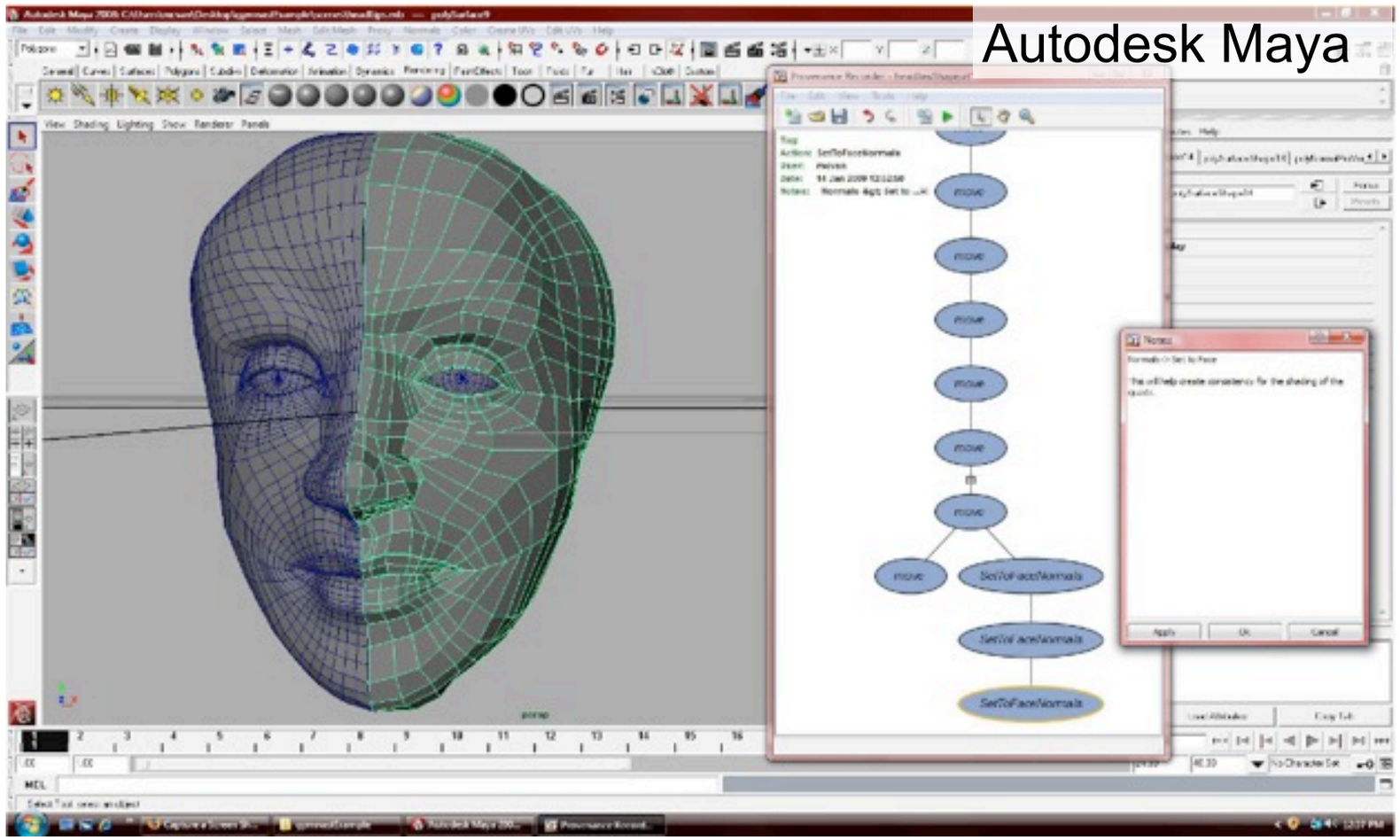
[VisTrails, Inc., IPAW 2008]

VisTrails Maya Plug-in



[VisTrails, Inc., IPAW 2008]

Provenance Enabling 3rd-Party Tools



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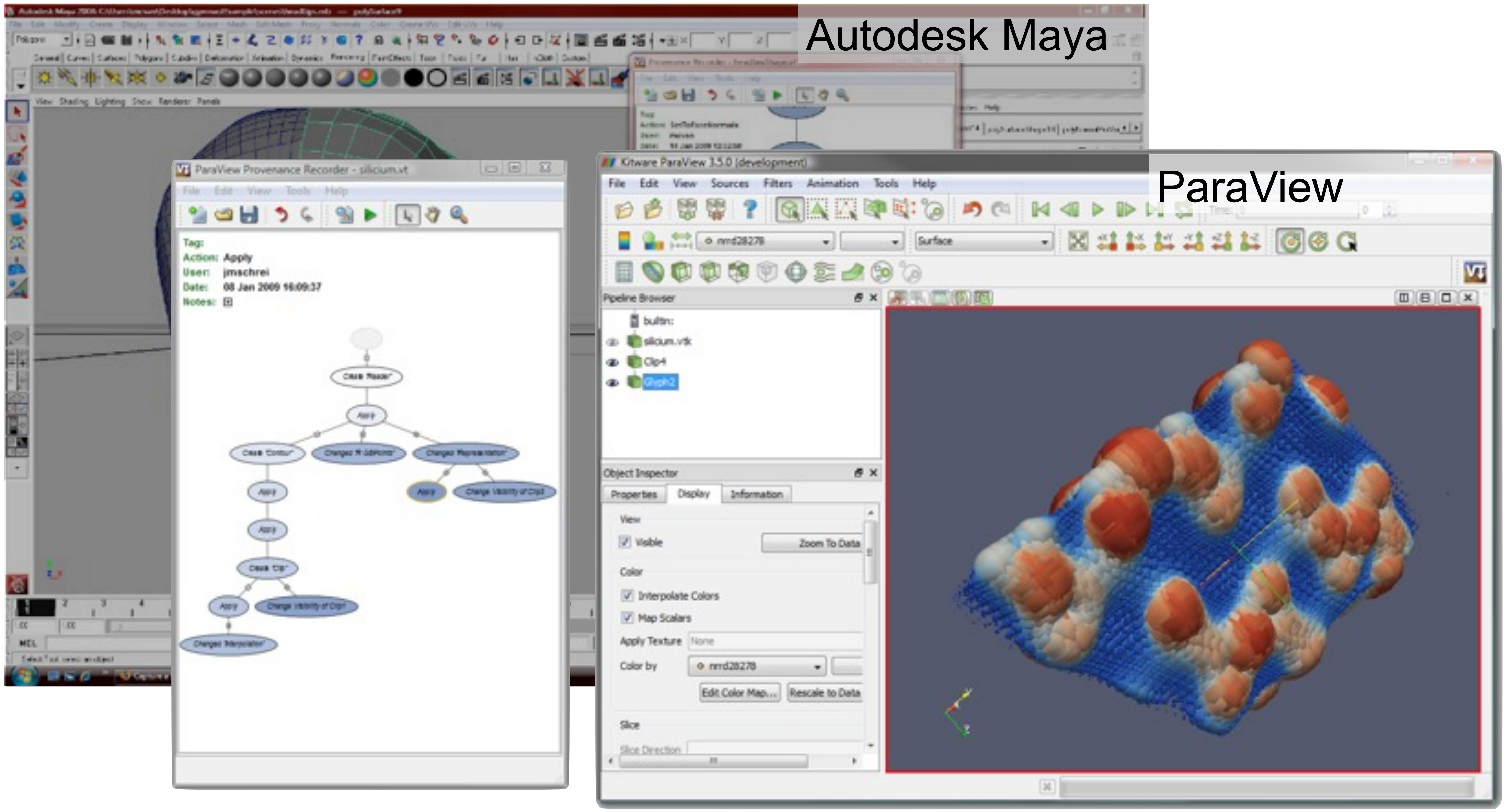

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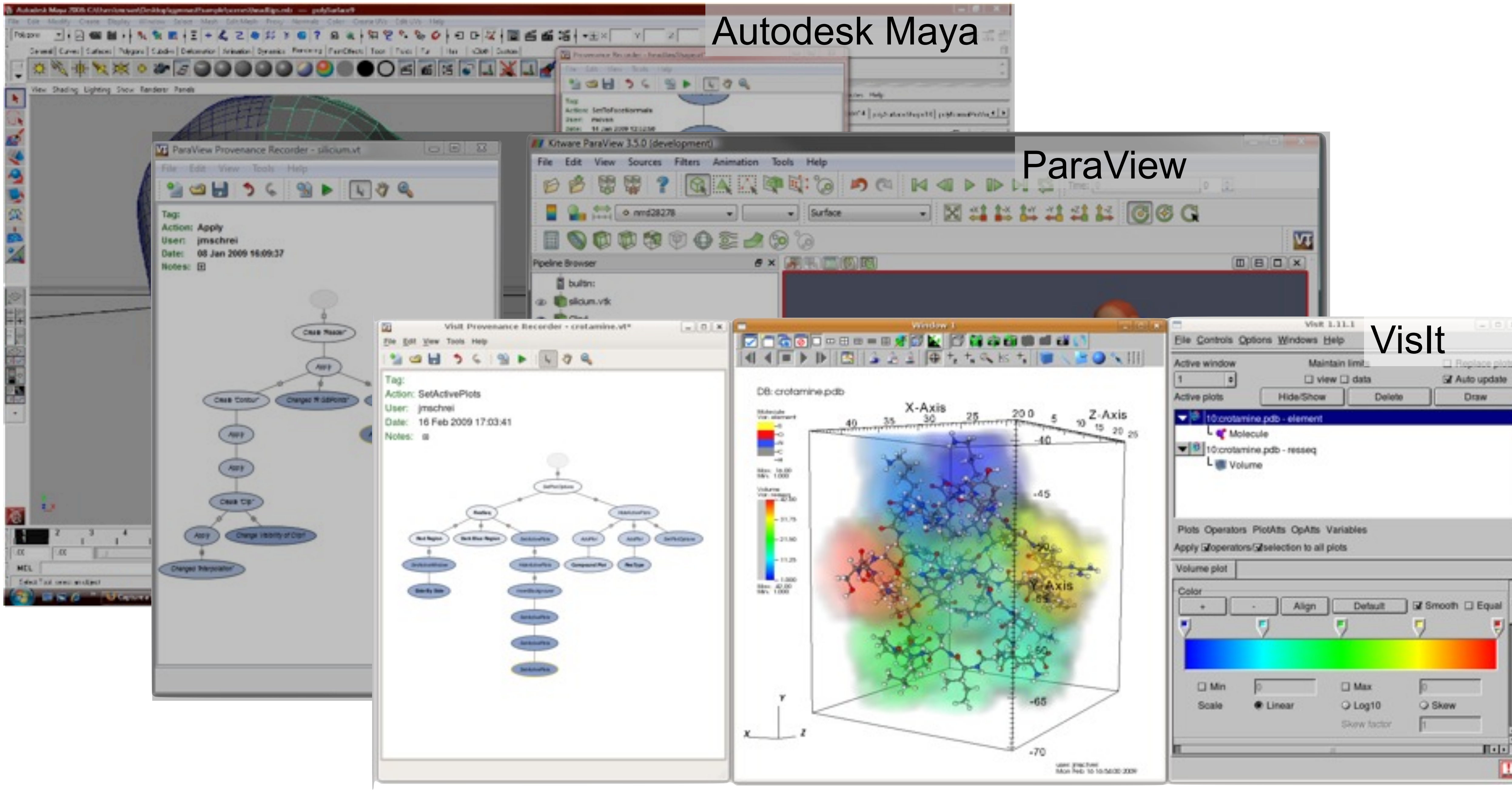
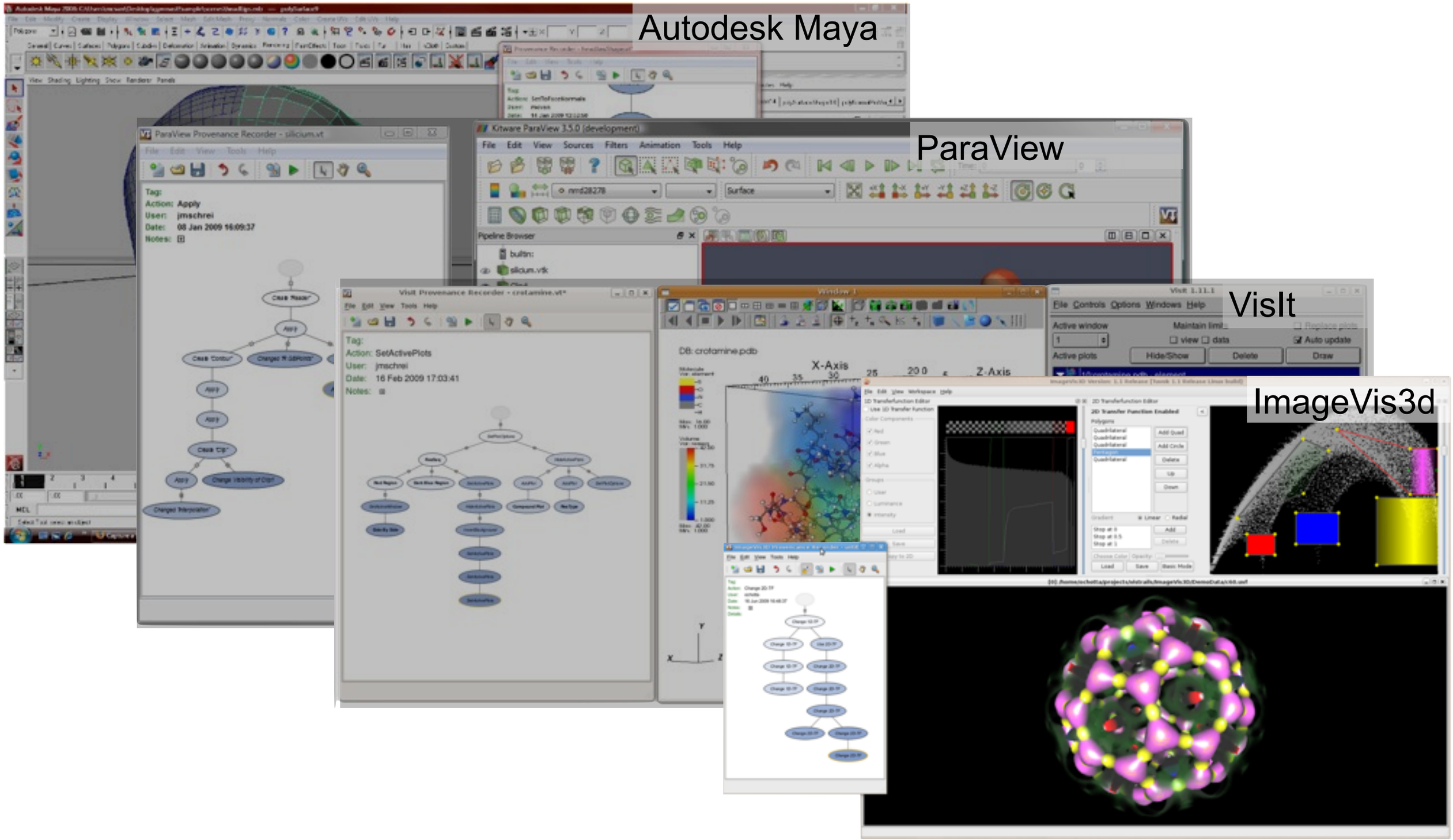


Friday, February 19, 2010

Provenance Enabling 3rd-Party Tools



Acknowledgments

- **Python Community**
- VisTrails Users & Developers
- VisTrails Team
  - Dr. Cláudio Silva
  - Dr. Juliana Freire

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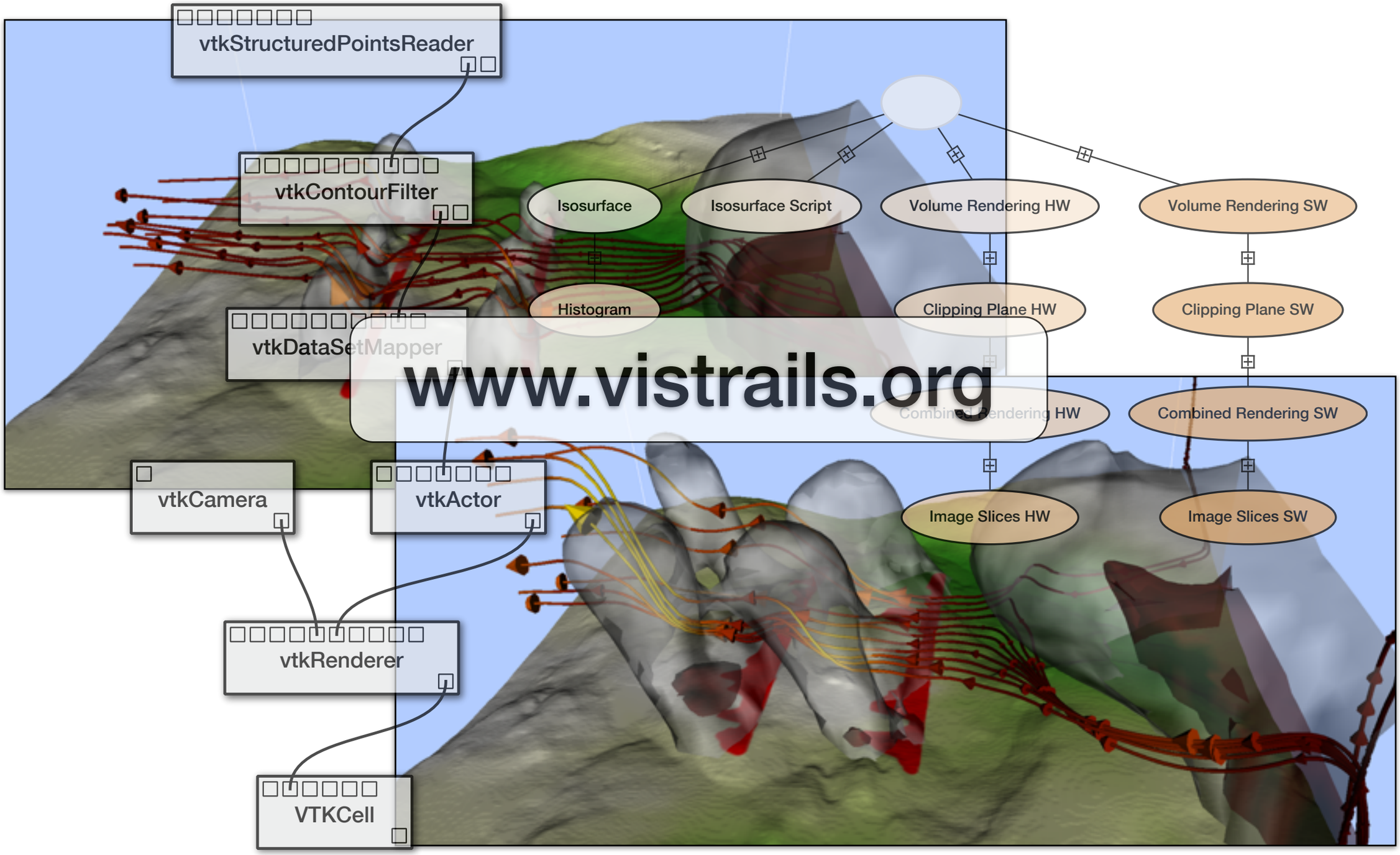
National Science Foundation WHERE DISCOVERIES BEGIN

Questions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vtkContourFilter
vtkDataSetMapper
vtkCamera
vtkActor
vtkRenderer
VTKCell
Isosurface
Isosurface Script
Volume Rendering HW
Volume Rendering SW
Histogram
Clipping Plane HW
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Combined Rendering HW
Combined Rendering SW
Image Slices HW
Image Slices SW
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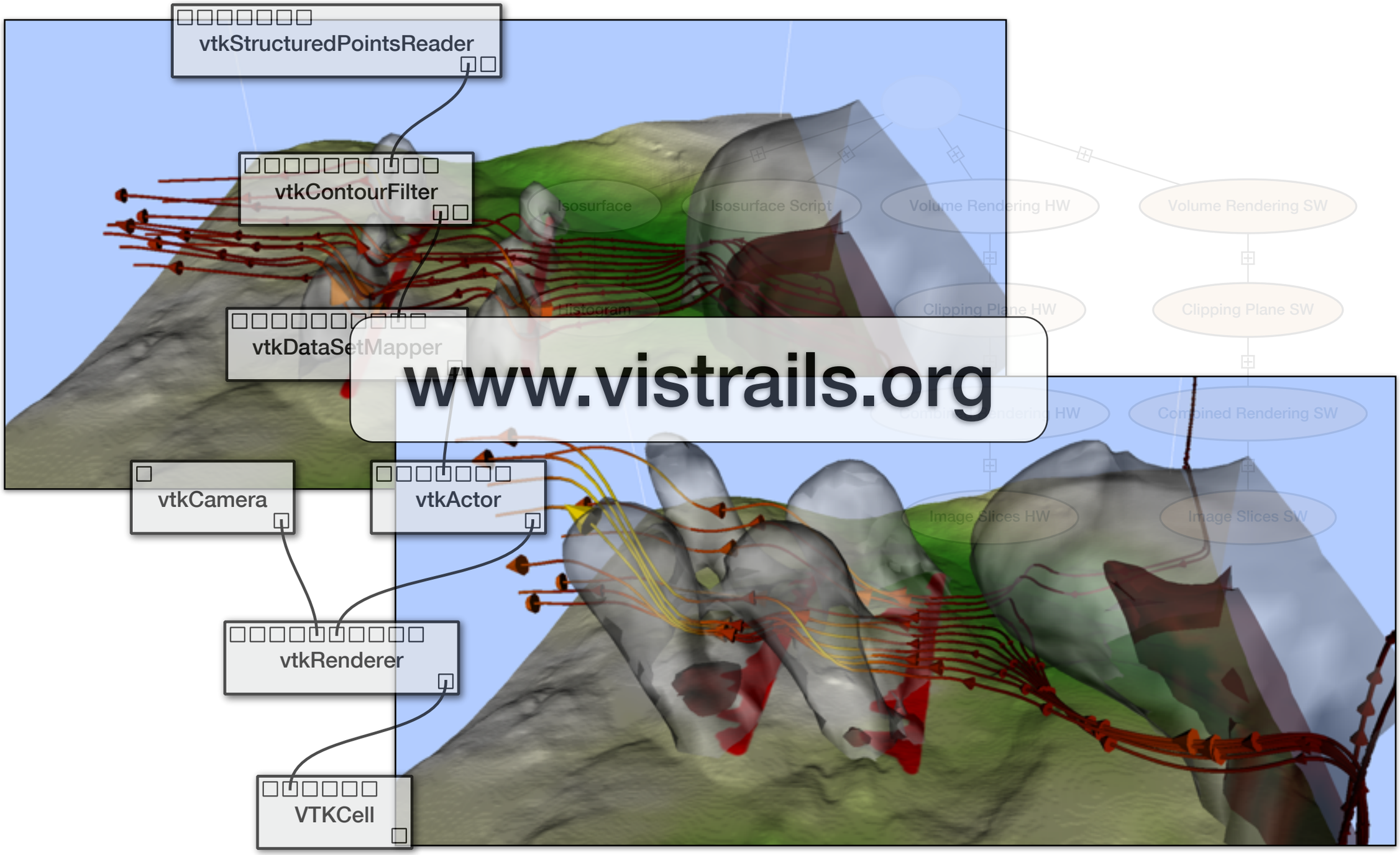
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